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ELECTROSTATIC ANALYSIS OF CHARGE-COUPLED STRUCTURES

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16. ABSTRACT

This report deals with the electrostatic analysis of various charge coupled structures. The analysis is based upon a numerical solution of Gauss's law for the multiple dielectric semiconductor and electrode structure. The formulation results in a large set of equations, usually non-linear, which are solved by an iterative scheme based upon the Gauss-Seidel method employing a relaxation parameter. Proper consideration of the non-linearity of the space-charge in the semiconductor allows convergent solutions which should give reasonable approximations to the channel potential profiles though not as good for estimating the space charge itself.

The results of this work are three programs which are listed in the Appendices. Section 1 discusses the analytical formulation and structures considered. Section 2 discusses the formulation of the non-linear space charge function. Section 3 discusses the three-electrode program and its application. Sections 4 and 5, respectively, are devoted to discussions of two and four electrode programs and their applications.

None of the programs give the electric field explicitly as output data. When this information is desired, the programs can be expanded to include field estimations based on a polynominal fit to the potential field, or they may serve as subprograms for main programs dealing with general aspects of charge transfer.

The concluding section deals briefly with the work which has been done on estimating charge transfer times for minority carriers.

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1. INTRODUCTION

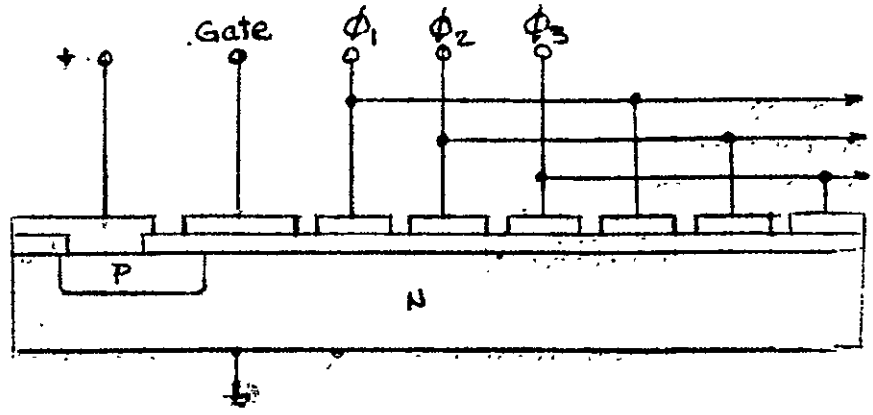
This report presents the results obtained in an investigation of charge-coupled shift register structures. The results which should be of use in analyzing CCD designs are computer programs which are described in Sections 3, 4, and 5. These programs allow one to obtain a two-dimensional electrostatic analysis of the CCD structure to determine if the structure allows the efficient transfer of charge. Features of significant interest are that two channel oxide thicknesses, two levels of metallization, and variable channel doping can be accommodated. The program presented in Section 3 can be used to analyze CCD input-output gates, and the program in Sections 4 and 5 can be used to analyze 2-phase structures with periodic boundary conditions.

The remainder of the report deals with the formulation of the analysis implemented by the programs. Factors which influence accuracy and rate of convergence are discussed.

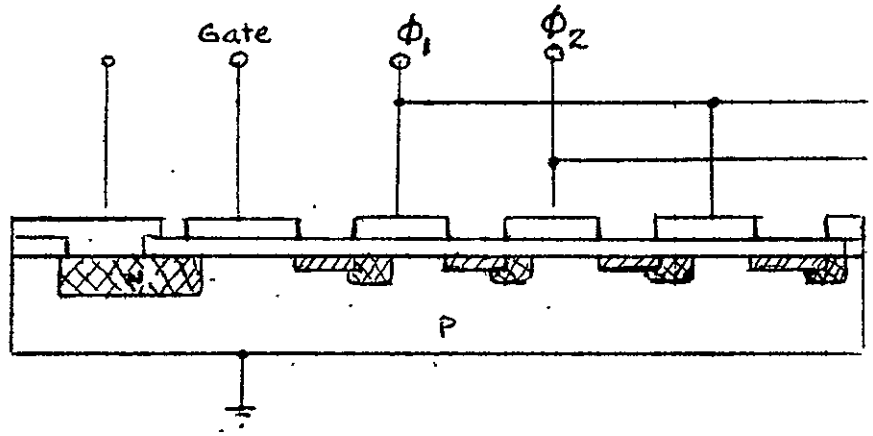
1.1 Structures of Interest

Figure 1.1 gives a two-dimensional diagram of a 3-phase structure discussed by Boyle and Smith[1,2] This structure originally was considered as having a uniform channel oxide thickness and uniform channel doping. Later, Walden, et. al.[3] considered the buried layer in which the doping varied from the $SiSiO_2$ interface into the substrate so that the maximum potential occurred below the interface.

Figure 1.2 illustrates a 2-phase structure reported by Krambeck, et. al.[4] in which shallow doping varies longitudinally along the channel. Variable doping can preclude problems of charge-trapping by fast-surface



1.1



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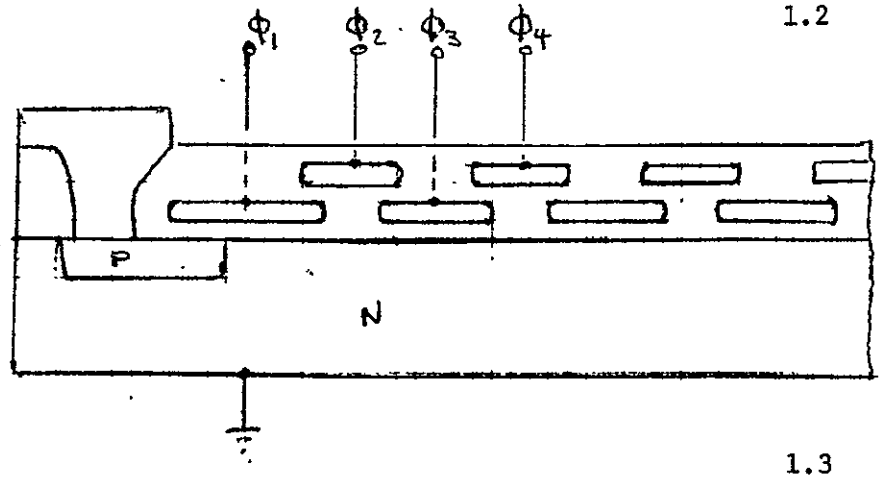

1.3

Some CCD structures.

states by forcing carriers away from the interface and also can preclude charge trapping due to potential barriers and wells in the gap and under electrode edges. Longitudinal variation of the doping can also give the potential asymmetry required for unidirectionality of the charge transfer. The benefits of these complications of the simple structure are discussed in the references cited.

Figure (1.3) illustrates a 2-phase structure with two-levels of metallization and multiple channel oxide thickness. In such a structure, overlapping electrodes preclude potential barriers such as may occur in an interelectrode gap. The multiple oxide thickness allows the required asymmetry for 2-phase operation. An added benefit, is that overlapping electrodes shield the channel from static charge which may accumulate on the surface of the oxide at the air-oxide interface, thus precluding unpredictable variations in the channel potential. Kosonocky and Carnes[5] have discussed this type of structure.

1.2 Ideal Mode of Operation

In this mode of operation the channel is depleted of minority carriers except those which are gated into the input end of the channel and transferred by the attractive potential produced by the transfer electrodes. At the edges of the channel, charge is confined by a potential barrier which arises naturally for an N-substrate device with a thick field oxide but must be produced by an N+ channel stop diffusion for P- substrate devices. The surface potential under an electrode is obtained from the MOS capacitor formula:

$$\psi_s = V_G - V_{FB} - \frac{Q_B + Q}{C_{OX}} \qquad (1.1)$$

The substrate charge Q_B depends upon ψ_S, the surface potential so that equation (1.1) becomes a quadratic which is easily solved for ψ_S. Q is the free-charge, and in the ideal mode of operation, it is small enough to neglect. A necessary condition for charge transfer is that the attractive potential of the succeeding electrode in the direction of transfer must exceed that of the preceding. In the ideal operating mode no barriers exist in the interelectrode gap and the necessary condition is also sufficient for transfer.

Equation (1.1) is also useful for estimating the amount of charge, Q, which can be accumulated under an electrode before the attractive potential is equal to that of the preceding electrode, i.e., the full well condition. The amount of charge injected into the channel from a junction by means of a control gate can be found in a like manner. Extension of the concept by integration allows an estimate of trapped charge when potential barriers occur in practical structures.

In practice, potential wells and barriers may exist and preclude complete charge transfer. Their occurrence depends upon the CCD structural parameters such as electrode geometry, oxide thickness and channel doping. Such phenomena must be investigated by two-dimensional analyses. Amelio[6] has pointed out the utility of analyzing an assumed ideal mode of operation. It is assumed that transfer can occur and that Q is sufficiently small to be negligible. Neglecting the minority carrier concentration allows the analysis to be carried out without simultaneous solutions of the current flow equations. The potential distribution calculated is valid for almost a clock period and is a steady-state solution provided that charge transfer keeps the channel depleted. If the solution shows potential barriers and wells, the

results provide a means for estimating the magnitude of the free charge which will be trapped in actual operation.

1.3 Formulation of the Two-Dimensional Electrostatic Analysis

The complexities which arise in considering a realistic model suggest a numerical approach. An approach based on Gauss' law is chosen because it allows the treatment of discontinuities in a straightforward manner. There are a number of these discontinuities, including those of the dielectric constant, of the conductivity, and those arising from surface charge distributions. A rectangular cell structure, such as illustrated in Figure 1.4, is most convenient for formulation of a discrete problem from a continuous one. The grid points within the cells are chosen to lie on the lines of discontinuity.

A formulation of Gauss' law for each cell should consider a rectangular cylinder of unit length, so that:

$$\oint_{C_{ij}} \vec{D} \cdot \vec{n} \, d\ell = Q_{ij} \tag{1.2}$$

$$Q_{ij} = \int_{S_{ij}} \int \rho \, dxdy + \int_{L} \sigma_L dx \tag{1.3}$$

where $\vec{D}$ is the electric flux density, ρ is the volume charge density, and σ_L is a line charge density which always occurs on a line parallel with the x-axis. This formulation is consistent with a two-dimensional analysis. The electric flux density is defined in terms of the electrostatic potential u by:

$$\vec{D} = - \varepsilon \nabla u \tag{1.4}$$

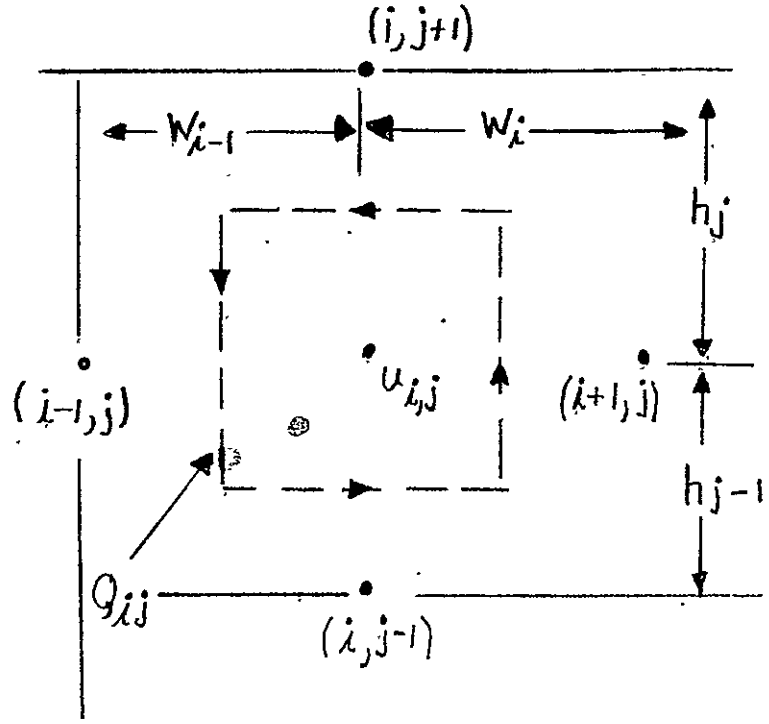

Figure 1.4 Discrete Cell

A two point finite difference formula is used to define the gradient along each boundary on the cell in all succeeding work. Obviously, higher order formulas could be used at the expense of increased computation time. Using a two-point formula and keeping in mind that the cell point is chosen to lie on any line of discontinuity passing through the cell, then one obtains for (1.2) evaluated on the cell:

$$\begin{aligned}
&\left(\frac{u_{i+1,j} - u_{i,j}}{w_i}\right)\left(\frac{\varepsilon_{j-1}\, h_{j-1}}{2} + \frac{\varepsilon_j\, h_j}{2}\right) \\
&+ \left(\frac{u_{i,j+1} - u_{i,j}}{h_j}\right)\left(\frac{\varepsilon_j\, w_{i-1}}{2} + \frac{\varepsilon_j\, w_i}{2}\right) \\
&+ \left(\frac{u_{i-1,j} - u_{i,j}}{w_{i-1}}\right)\left(\frac{\varepsilon_{j-1}\, h_{j-1}}{2} + \frac{\varepsilon_j\, h_j}{2}\right) \\
&+ \left(\frac{u_{i,j-1} - u_{i,j}}{h_{j-1}}\right)\left(\frac{\varepsilon_{j-1}\, w_{i-1}}{2} + \frac{\varepsilon_{j-1} w_i}{2}\right) = -Q_{ij}
\end{aligned} \tag{1.5}$$

Generally determining Q_{ij} requires averaging ρ over the cell and consideration of the fact that ρ depends in a non-linear manner on the potential. Furthermore, σ_L, which will have a specified spatial distribution, must be averaged over the line. These points are considered in detail later.

Equation (1.5) is rewritten in the form given by (1.6) which is the typical equation for a nonlinear set.

$$-A_{i,j}u_{i,j-1} - B_{i,j}u_{i-1,j} + C_{i,j}u_{i,j} - D_{ij}u_{i+1,j} - E_{ij}u_{i,j+1} = Q_{ij}(u_{i-1,j}, u_{i,j-1}, u_{i,j}, u_{i+1,j}, u_{i,j+1}) \tag{1.6}$$

The solution of this set of equations gives an approximation of the potential at grid points in the field. It may be noted that for certain schemes for finding Q_{ij}, equation (1.6) is equivalent to the finite difference approximation to Poisson's equation used by Amelio[6].

1.4 Survey of Difficulties in Obtaining a Solution

The major problem is in finding a scheme for solving the large system of equations. A secondary, but also important problem is in finding Q_{ij} Closely associated with the latter problem is choosing cell sizes which give suitable accuracy.

Let us assume the grid has $N_T = M \times N$ points. Then equation (1.6) defines a set of N_T equations. Typically this number may range from 2000 to 10,000 points. Systems of non-linear equations may be solved by the Newton-Raphson approach[7] which involves the iterative solution of a set of linear equations in an incremental potential $\delta u_{i,j}$ until all $\delta u_{i,j}$'s are reduced to a suitably small value. However, the resulting

set of linear equations is so large typically, that an iterative scheme must be used to solve the linear set. Therefore, the scheme may become prohibitively expensive if some alternate method will work. This consideration led us to consider the application of the Gauss-Seidel method[8] directly to the non-linear system.

The matrix equation may be written as:

$$[A]\,[u] = [Q] \tag{1.7}$$

Assume for the moment that $[Q]$ is independent of $[u]$, which would be in fact true except within the semiconductor and on conducting boundaries which will be excluded. The Gauss-Seidel method for solving such a system is an iterative scheme which gives the $(n+1)^{th}$ approximation of u_I as:

$$u_I^{(n+1)} = -\frac{1}{a_{II}} \sum_{J=1}^{I-1} a_{IJ} u_J^{(n+1)} - \frac{1}{a_{II}} \sum_{J=I+1}^{N_T} a_{IJ} u_J^{(n)} + \frac{Q_I}{k_I} \tag{1.8}$$

where the single subscript (I) is related to the double subscript (i,j) by:

$$I = (j - 1)M + i \tag{1.9}$$

and,

$$N_T = M \times N \tag{1.10}$$

We do not have assurance that this scheme will converge for a non-linear set. (In fact, we have had experiences where it did not which are discussed later.) For a linear set, the scheme can be made convergent by suitable choice of a relaxation parameter, ω. For $\omega < 1$, the method is referred to as under-relaxation and for $\omega > 1$

over-relaxation. In either case, we have:

$$u_I^{(n+1)} = u_I^{(n)} + \omega[\tilde{u}_I^{(n+1)} - u_I^{(n)}] \tag{1.11}$$

where $\tilde{u}_I^{(n+1)}$ is given by (1.8). The problem here is with convergence and obtaining a suitably rapid rate to preclude excessive computing time. There is no problem with round-off errors. (See Westlake[9].)

Several factors must be considered in the choice of the grid size. It can be shown that the differencing scheme used here leads to second order accuracy, so that differencing errors are of order $0(h^2 + w^2)$. The effect of changing the grid size on the differencing error could be easily investigated experimentally. However, the effect of the grid size in determining Q_{ij} requires some analytical consideration and is treated in detail in Section 2.

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2. ONE-DIMENSIONAL MODELS OF AN MIS STRUCTURE

The simple one-dimensional structure is useful for analysis in order to determine the effect of grid spacing along the y direction in the silicon substrate on the accuracy of numerical solutions. Very accurate one-dimensional solutions can be obtained without excessive computer time. Furthermore, the physical picture is simpler, and this aids in choosing useful models for calculating the charge density.

2.1 The Depletion-Layer Model

This model is well known and has proved to be quite useful.[1] It is illustrated in Figure 2.1, which shows the charge distribution assumed. On the silicon side of the Si-SiO_2 interface, the free minority charge is assumed to be accumulated with a surface charge density Q. Also present on the oxide-side is the fixed surface stat charge Q_{ss}. Below the surface is a depletion layer extending to a depth $y = - y_d$. The surface normal field in the semiconductor E_s and the interface potential ψ_s are obtained from Poisson's equation.

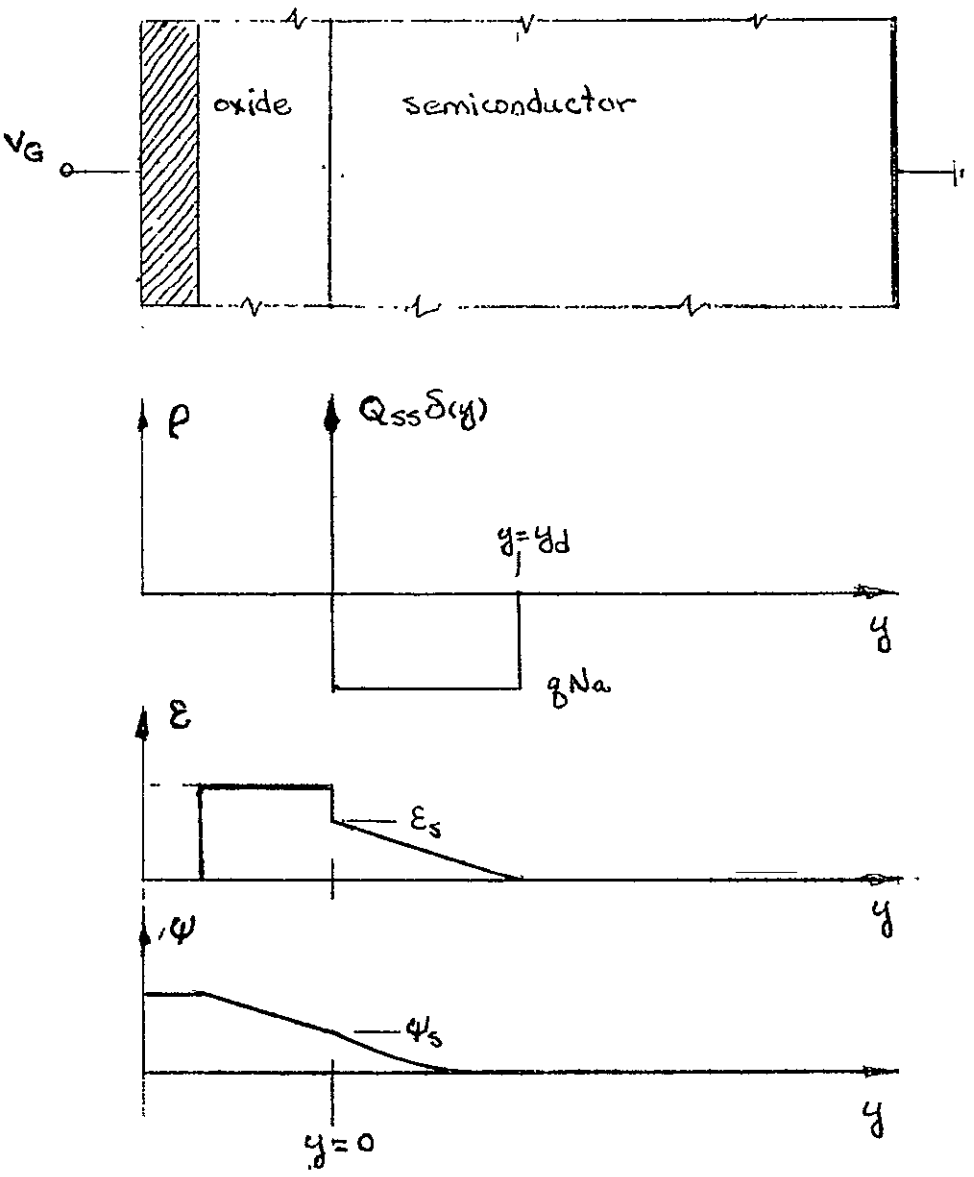
$$E_s = + \frac{qNa}{E_s} y_d \tag{2.1}$$

$$\psi_s = \frac{1}{2} \frac{qNa}{E_s} y_d^2 \tag{2.2}$$

The potential in the semiconductor with respect to the bulk is:

$$\psi(y) = \frac{1}{2} \frac{qNa}{\varepsilon_s} (y - y_d)^2 \quad 0 \leq y \leq + y_d \tag{2.3}$$

Applying Gauss's law at the interface to obtain the field in the oxide:



2.1 Space Charge, Field, and Potential for MOS Structure based on Depletion Layer Theory.

$$D_{ox} = \varepsilon_s E_s - Q_{ss} - Q \tag{2.4a}$$

$$E_{ox} = \frac{\varepsilon_s E_s}{\varepsilon_{ox}} - \frac{Q_{ss}}{\varepsilon_{ox}} - \frac{Q}{\varepsilon_{ox}} \tag{2.4b}$$

Integrating to obtain the gate potential and ignoring the oxide charge and the contact potential of the metal-semiconductor contact, the gate potential V_G is:

$$V_G = (qN_B y_d - Q - Q_{ss}) \frac{\varepsilon_{ox}}{\varepsilon_{ox}} + \psi_s \tag{2.5a}$$

$$V_G = \frac{Q_B - Q - Q_{ss}}{C_{ox}} + \psi_s \tag{2.5b}$$

$$C_{ox} \triangleq \varepsilon_{ox}/\varepsilon_{ox} \text{ , oxide capacitance.} \tag{2.5c}$$

Equations (2.2) and (2.5) are useful for making estimates of the performance capabilities of MOS structures.

2.2 Equilibrium Models

In a more exact solution the hole-electron concentration would be allowed to vary continuously according to equilibrium relations:

$$p = n_i e^{-q(\psi - \phi_p)/kT} \tag{2.6a}$$

$$n = n_i e^{q(\psi - \phi_n)/kT} \tag{2.6b}$$

where ϕ_p and ϕ_n are the quasi-fermi potentials for holes and electrons and ψ is the electrostatic potential defined to be zero at the point where $p = n = n_i$ in thermal equilibrium.

Unfortunately, the current flow and continuity equations must generally be simultaneously solved in order to find ϕ_p and ϕ_n

However, let us consider a transient situation in which a voltage is applied to the gate and consider a time interval beginning at a time substantially greater than the relaxation time but shorter than the excess carrier lifetime. The majority carriers are repelled from the interface and minority carriers are attracted. Since equation (2.2) should be a reasonable approximation, we may conclude that the minority carriers are exponentially distributed in a very thin region near the interface provided the current density is small. Thus in the substrate at a small distance from the interface, Poisson's equation may be writte in terms of $\psi^1 = \psi - \psi_{(\text{substrate})}$ as:

$$\frac{d^2\psi^1}{dy^2} = \frac{-q}{\varepsilon}\left(N_a e^{-\frac{q\psi^1}{kT}} - N_a\right) \tag{2.7}$$

Normalizing, ψ^1 by kT/q, and y by the extrinsic deBye length $kT\varepsilon/q^2N_a$, we have:

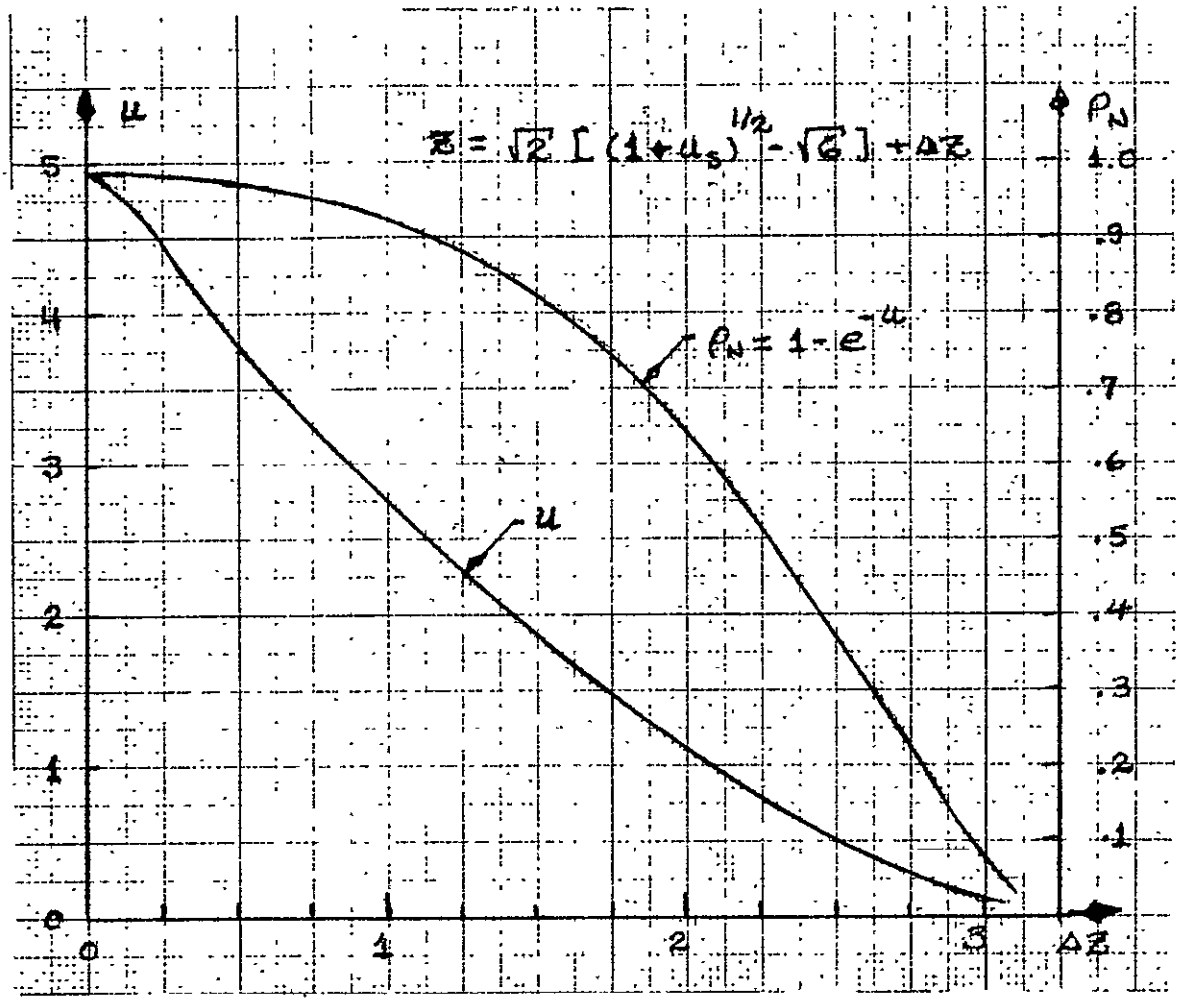
$$\frac{d^2u}{dz^2} = 1 - e^{-u} \tag{2.8}$$

Defining the normalized field by, $V = \frac{du}{dz}$, we may integrate (2.8) to obtain:

$$V^2 = 2u + 2(1 - e^{-u}) \tag{2.9a}$$

$$Z = \int_u^{u_s} \frac{d\eta}{\sqrt{2}\,(1 - e^{-\eta} + \eta)^{1/2}} \tag{2.9b}$$

The last term in (2.9a) is the deviation from the depletion layer approximation. In most cases of interest the surface potential will satisfy $u_s >> 1$. Suppose $u_s > 5$. The integral in (2.9b) can be broken down into two parts:



2.2 Normalized Potential and Space Charge Profile for Equilibrium Approximation.

$$Z \cong Z_1 + \Delta Z \tag{2.10a}$$

$$Z_1 = \int_s^{u_s} \frac{d\eta}{\sqrt{2}(1+\eta)^{1/2}} \tag{2.10b}$$

$$\Delta Z = \int_u^{u_s} \frac{d\eta}{\sqrt{2}(1-e^{-\eta}+\eta)^{1/2}} \tag{2.10c}$$

Figure (2.2) shows the variation of u with respect to Z and also the normalized charge density, $(1 - e^{-u})$. Let us check the case $\psi_s = 1$ volt, $u_s = 38.61$. The depletion approximation gives $Z_d = 8.787$, which would correspond to $\Delta Z = 3.351$.

Numerical solutions require consideration of a finite region. When we consider applying the preceding models in numerical analysis, obviously there will be a significant difference between the ratio of the charge to surface potential if we consider interface voltages as low as 1 volt. This ratio, r, of the substrate charge for an equilibrium distribution to that for a depletion layer approximation is:

$$r \cong \frac{(1+u_s)^{1/2} - .858}{(u_s)^{1/2}} \tag{2.11}$$

If one were considering the effects of the surface state charge Q_{ss} alone in the absence of an electrode, then significant errors may result from the depletion approximation, particularly if the resultant potential is low. However, in this case the absolute error is also lowered. This feature seems to save the depletion approximation from failure when otherwise it appears grossly in error.

The space charge density changes from 95% to 5% of its maximum value in approximately 2.3 extrinsic deBye lengths. Therefore, we conclude

that a space charge-potential function model which shows a continuous variation will be of significance in a numerical analysis only if the grid size, h, is less than an extrinsic de Bye length. This conclusion is important because it is typically expensive in terms of grid points to maintain the grid size at this small a value along the depletion edge.

2.3 Choice of Grid Size and Boundary

The boundary value problem for an MIS structure is most easily formulated as one of infinite or semi-infinite extent. Practically, substrate thicknesses are much larger than depletion depths. Since a finite region must be considered, one must choose a suitable boundary. The boundary should be reasonably distant from the region in which the potential gradient varies significantly.

If economy of storage and running time on the computer is paramount, this choice of a boundary should be a subject for careful investigation. We have chosen the boundary on which the potential is specified ($u = 0$) at a distance of twice the estimated depletion depth for first solutions. By monitoring solutions one confirms that this indeed removes the boundary far enough away; however, it shows that a significant amount of the total storage for data points is seldom used.

The number of points used in the grid can be reduced if one chooses a variable grid size. This must be done with care or significant errors will result. In the following, we will estimate errors which may occur due to round off or quantization of the charge in a cell assuming only two charge density levels. Other schemes for averaging the space charge may reduce these errors.

We choose the boundary at which $u = 0$ for a maximum surface potential, $U_s(MAX)$, at a distance $2Z_d(MAX)$, where using a depletion approximation:

$$Z_d(MAX) = \sqrt{2\, U_s(MAX)}$$

We allow a total of N points to span the distance $2Z_d(MAX)$ spaced at $(Z_1, Z_2, \cdots Z_N)$. Using a depletion approximation, we have:

$$\frac{\Delta U_s}{U_s} = 2\,\frac{\Delta Z_d}{Z_d} \tag{2.12}$$

where Z_d is the depletion depth corresponding to any U_s. We assume that the resolution will be one-half of a cell:

$$\Delta Z \cong (Z_{n+1} - Z_{n-1})/4$$

Therefore:

$$\frac{\Delta U_s}{U_s} \cong \frac{Z_{n+1} - Z_{n-1}}{2Z_n} \tag{2.13}$$

Let us assume a uniform grid, $Z_n - Z_{n-1} = h_o$, then:

$$\frac{\Delta U_s}{U_s} \cong \frac{1}{n} \tag{2.14}$$

The percentage error decreases the further the depletion layer extends. However, the absolute value of the error increases:

$$\Delta U_s \cong n\, h_o^2$$

For example, if we choose 50 points to span the grid and estimate that the maximum error occurs at $n \doteq 25$, then we obtain a percentage error of about 4%.

Let us use (2.13) to define a grid with uniform percentage error of 100a. This leads to a difference equation:

$$Z_{n+1} - 2aZ_n - Z_{n-1} = 0 \qquad (2.15)$$

with a solution:

$$Z_n = h_o \alpha^{n-1} \qquad (2.16a)$$

$$\alpha = a \pm \sqrt{1 + a^2} \qquad (2.16b)$$

$$\alpha \cong 1 + a \qquad (2.16c)$$

where in (2.16c) we require an expanding grid and note that a is small so that $a^2 << a$. The absolute error is:

$$\Delta U_s \cong \frac{(\alpha^n - \alpha^{n-2})}{4} h_o^2$$

Thus, it increases exponentially.

Now let us consider a case of interest where a maximum surface potential of approximately 20 volts must be accommodated. Using the uniform spacing of 50 points for $Z_d(MAX) \cong 40$, we would have $h_o = 2 \times 40/50 = 1.6$ deBye lengths. The maximum error would be approximately .8V at the surface with a percentage error of 4%.

Let us now determine the exponential spacing which preserves the same error under the high potential surface. We choose α and N to maintain this error to within 1 deBye length of the surface; i. e., $h_o = 1$. This would require approximately 113 points, of which 94 would be within the depletion distance. Changing h_o to 2 deBye lengths gives 94 points of which 77 would be within the depletion region. Further division of the grid within the first exponential step would cost even more points.

Any non-uniform spacing which preserves the accuracy for high potential at lower potentials will require more points in the grid. The grid points may be better utilized (i.e., fewer zeros stored) with the non-uniform grid. However, there is another consideration which weighs heavily against compromising the accuracy of solutions for higher surface potential to obtain accuracy for lower potentials.

In analyzing a CCD structure, the differences in potential along the interface will be of great interest. It will be essential to preserve accuracy in finding the potential in the high potential region; otherwise, a relatively small percentage error in this region may lead to a relatively larger error in the potential gradient along the surface than the same percentage error at a region of lower potential.

The conflicting requirements for accuracy when the depletion region is both deep and shallow and the need to economize the number of grid points led us to a compromise. The larger region of the grid is uniformly spaced, extending a distance of $K \cdot x_d$, where the first run value for K is 2. Subsequent runs may reduce K if too large a portion of the field is unused. This uniform grid will have cell height typically between 1.5 and 3 deBye lengths, although by some experimentation it can sometimes be reduced to less than a deBye length without an excessive number of points. This uniform grid is spliced into an exponential grid extending from the surface to a distance of N_d deBye lengths, defined by:

$$h_n = h_o \alpha^{n-1} \tag{2.17a}$$

$$Z_n = \sum_{k=1}^{n} h_k = h_o \left(\frac{\alpha^n - 1}{\alpha - 1}\right) \tag{2.17b}$$

Choosing, $\alpha = 1 + a$, where a is small, we obtain a fractional error which is 1 for $n = 1$ and approaches the value "a" for large n. For the examples which we have considered with doping between 10^{14} and 5×10^{15}, oxides from .1 to .5 μ, and voltages from -1 to 20 volts, we have observed that the depletion layer is usually at least 10 deBye lengths from the surface. The uniform grid usually insures maximum errors in the range of 10 - 30%. Now in order to make a smooth transition across the interface, i. e., no large changes in coefficients of the equations for u_{ij}, we require h_o to take certain values related to the grid size in the oxide. These values, in deBye lengths, range from .375 (low doping) to 2 (high doping). In the former case approximately 37 points are required to extend 10 deBye lengths and obtain 10% error bound. In the latter case, these requirements are incompatible and the exponential grid is not used. Thus far we have used an exponential grid which extends 2 deBye lengths.

We have discussed in detail the effect of grid size on round-off error, assuming that binary values can be assigned in each cell half. The grid size of course affects the solution otherwise, depending upon the order of the differencing schemes used. We have used the previous considerations to aid in choosing the grid scheme, and then we have experimented with the grid size, halving and quartering it, to determine the effect upon convergent solutions. When these solutions are in agreement, we feel the techniques produce numerical results at least as good as the model, and, consequently, of use in determining design feasibility.

Reference

1. A. S. Grove, Physics--Semiconducting Devices, Chap. 9, Wiley, 1967.

3. TWO-DIMENSIONAL ANALYSIS OF 3-ELECTRODE STRUCTURE

The 3-electrode structure is illustrated in Figure 3.1, and it could be considered as a storage cell for a 3-phase CCD structure or as a gating structure for a CCD or SCT (surface charge transistor). A zero potential boundary encloses the structure to obtain a finite region for analysis. The effect of the location of this boundary can be determined empirically. The program given in Appendix A for analyzing this structure is based on the Gauss-Seidel iteration procedure modified by use of a relaxation parameter. The programmed formulas are:

$$\tilde{u}_{i,j}^{(n+1)} = \frac{A_j u_{i,j-1}^{(n+1)} + B_j u_{i-1,j}^{(n+1)} + B_j u_{i+1,j}^{(n)} + G_j u_{i,j+1}^{(n)} + Q_{i,j}}{C_i} \tag{3.1}$$

$$u_{i,j}^{(n+1)} = (1 - \omega)\, u_{i,j}^{(n)} + \omega\, \tilde{u}_{i,j}^{(n+1)} \tag{3.2}$$

where:

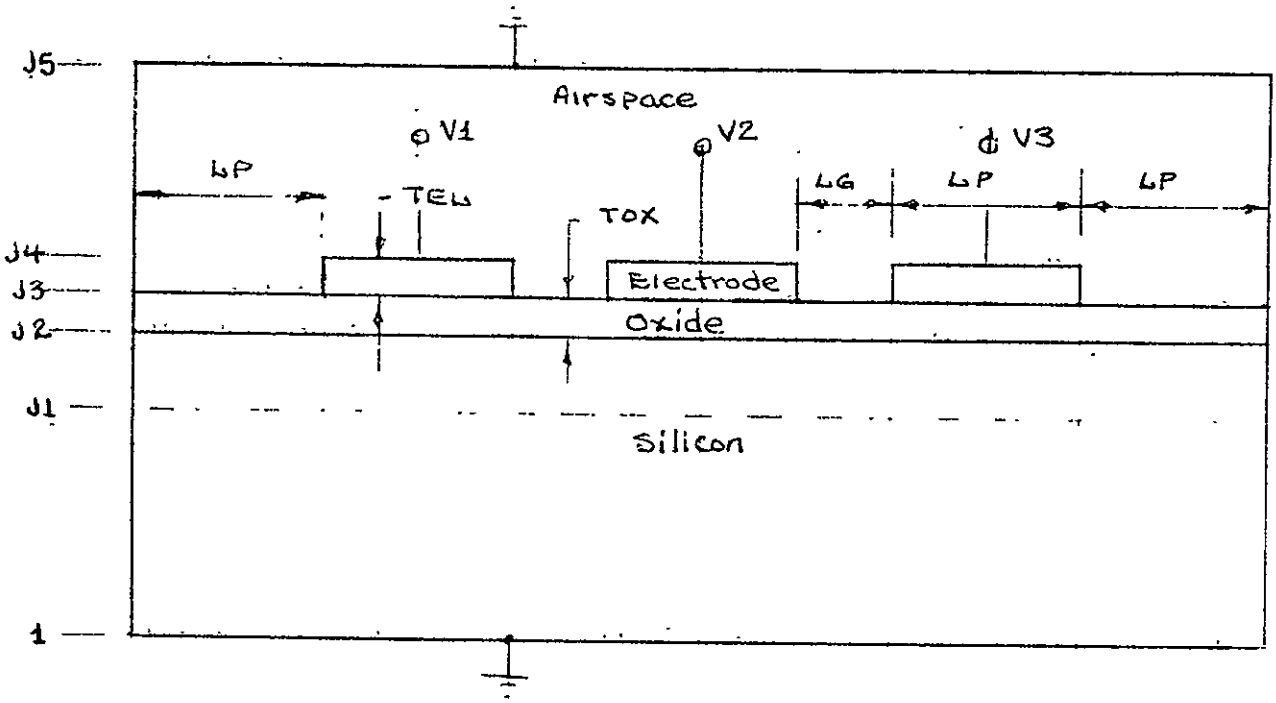
$$A_j = \varepsilon_{j-1}\, w/h_{j-1} \tag{3.3a}$$

$$B_j = (\varepsilon_{j-1}\, h_{j-1} + \varepsilon_j\, h_j)/2 \tag{3.3b}$$

$$G_j = \varepsilon_j\, w/h_j \tag{3.3c}$$

$$C_j = A_j + 2B_j + G_j \tag{3.3d}$$

The iterative procedure starts one line from the bottom boundary and one line to the right of the left boundary. It continues to the right along a row, then back to the left and upward. All points are considered except those at which the potential is fixed. After the field is swept through, the procedure is repeated until satisfactory convergence is



3.1 Three-Electrode Structure.

obtained. The coefficients in (3.3) are in fact calculated from the relative dielectric constants and Q_{ij} is divided by ϵ_o the free space permittivity.

We have not used a variable x-grid spacing although this is simple to accomplish. This can be done easily by modifying the subroutines COEFF and RELAX. However, it will require the operation of COEFF at each point rather than once for each line. This will considerably increase computation time, and, in our opinion, unnecessarily so for most purposes.

The cell charge in the substrate, Q_{ij} , is calculated using the subroutine AVERO. Several algorithms were evaluated and will be discussed in subsection 3.2

3.1 Grid Spacing

As mentioned above a uniform x-grid was used with various values for w evaluated. Figure 3.2 illustrates the y-grid spacing parameters. Spacing, through the electrodes and oxide are uniform with ratios roughly equal to the ratio of the dielectric constants. Above the electrodes the spacings are exponentially increased, with the spacing through the electrodes serving as the exponential base.

The spacing through the oxide serves as the base for the spacing in the substrate immediately below the interface. The basic step size is:

$$h_o = (t_{ox}/L3)(\epsilon_s/\epsilon_{ox}) .$$

Steps are exponentially spaced for a distance of 2 or more extrinsic deBye lengths. These exponential steps are calculated by the subroutine

YSPAC. The objectives in choosing this spacing were two-fold. First, it is desirable to match the coefficients A_j and G_j, which are large, on the boundary of the $Si-SiO_2$ interface. Second, we would like to increase the accuracy of computing Q_{ij} on the depletion edge for shallow depletion when it is possible to do so without compromising the accuracy on a deep depletion edge. The spacing below this region is uniform because uniform spacing spans the largest distance with the smallest maximum spacing, an obvious but important point when considering calculation of Q_{ij} on a deep depletion edge. The program sets the cell size equal to a constant, whose default value is 2, times the maximum depletion depth (estimated) divided by an integer (input data). We have used values of 25 and 50 for the integer.

3.2 Calculation of Q_{ij}

Several algorithms were tried for AVERO. The first one utilized the exponential dependence on u of ρ, the majority carrier approximation, discussed in Section (2). The average potential in each quarter of a cell was used, and the sum of the charges in the four quarters obtained. The average of top and bottom halves were used similarly, and then, finally, the average of the cell used.

There were difficulties with all these methods. First, when many iterations are required for convergence, i.e., starting with a poor approximation, oscillations of the potential in the substrate occur. Once the potential changes sign, large change in the exponential may occur. Reduction of the relaxation parameter damps this oscillation but slows convergence. If the exponential is made to depend on the negative of the potential magnitude, a new type of phenomena occurs which

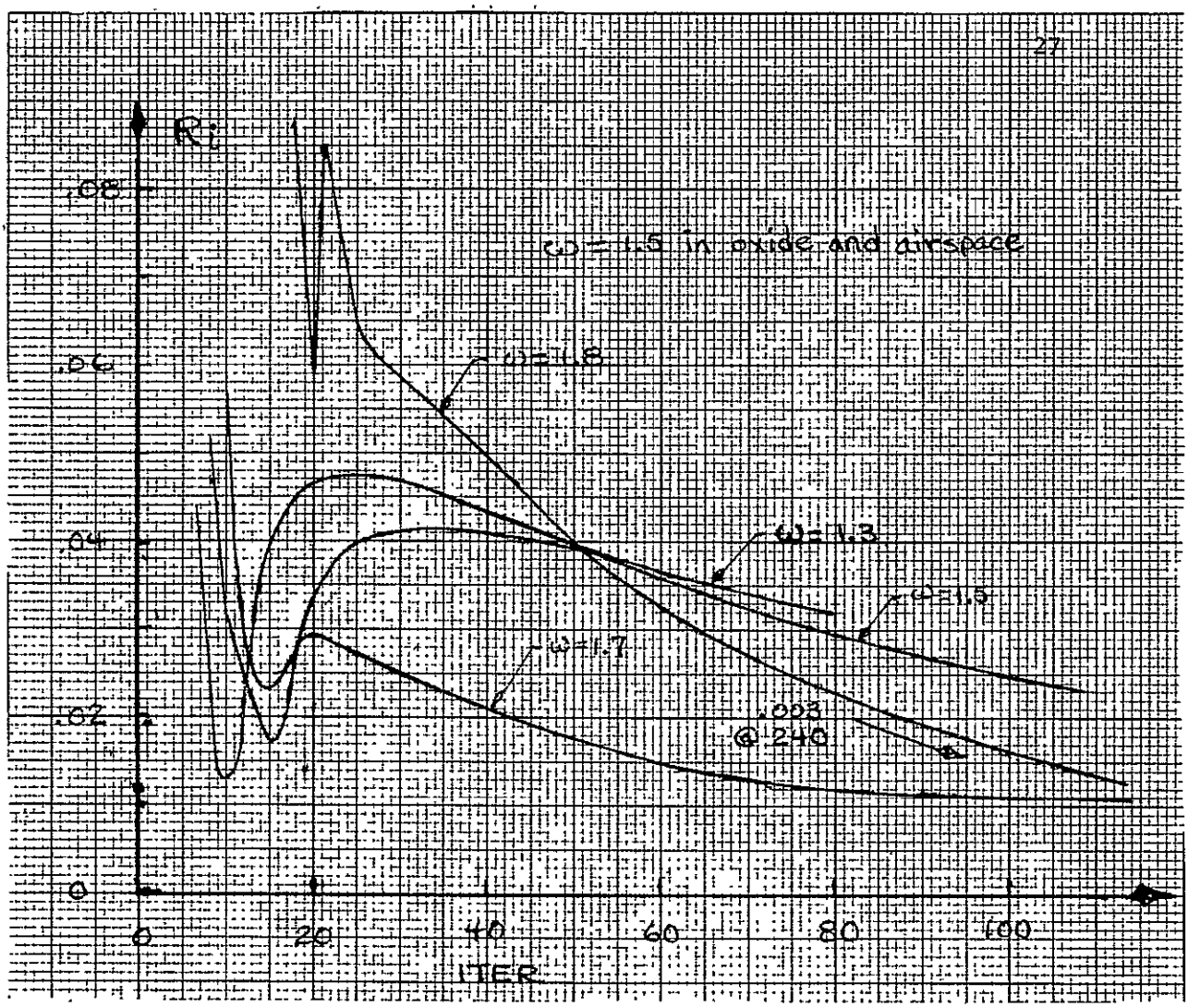
is worse. The depletion edge continues to advance with a negative dip in the potential (for a p-substrate) occurring. A stable solution will finally be obtained, which is obviously useless, where all the substrate is depleted.

The cure for the problem is to preclude the substrate potential from taking the wrong sign. When this step is taken, we find that the results obtained with an exponential function does not, in most cases, warrant the increased computing time. However, as pointed out earlier in section (2), it must make a difference when the depletion depth is shallow compared with an extrinsic deBye length. In most cases, we have used a simpler averaging technique involving binary values for the top and bottom of the cell. Whether binary or exponential weights are used, it makes little difference whether averaging is done on the right and left sides of the cell.

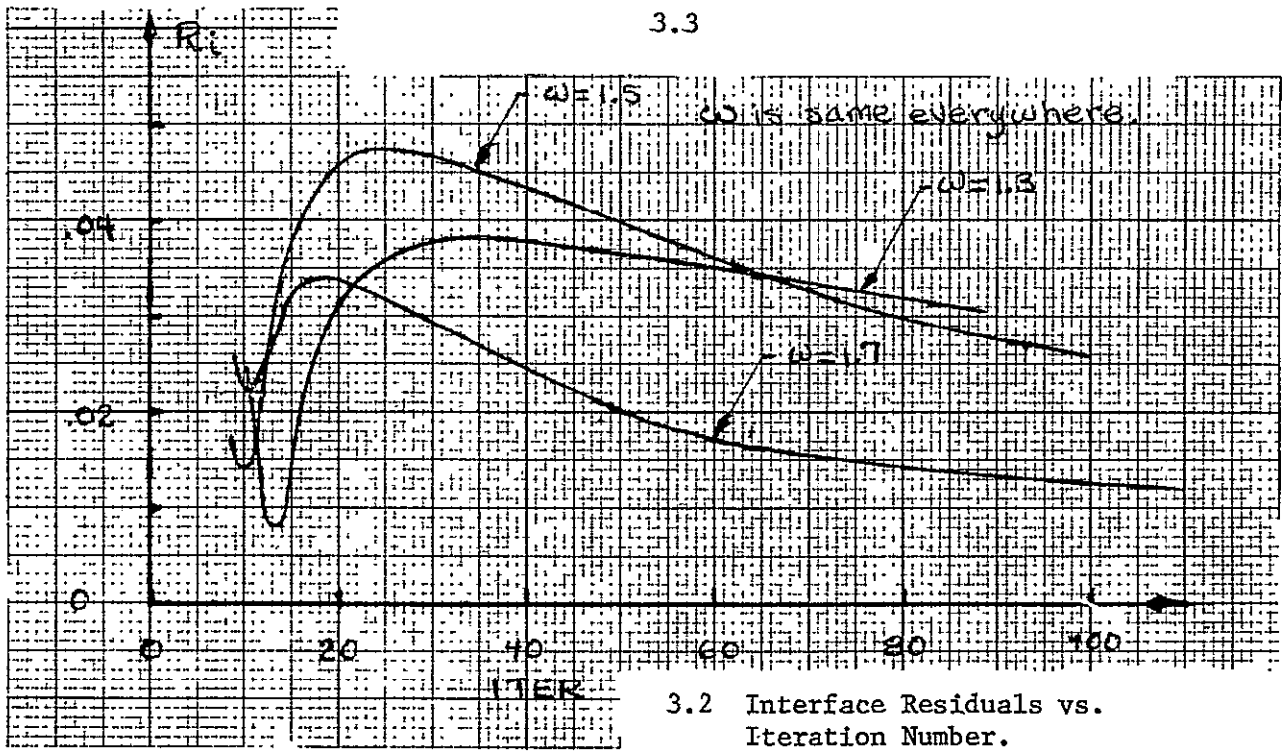
When the interface is considered, then the surface state charge Q_{ss} must be included as well as any charge due to shallow doping. The shallow doping varies along the channel, and averaging on the right and left hand sides of the cell should be done.

3.3 Convergence

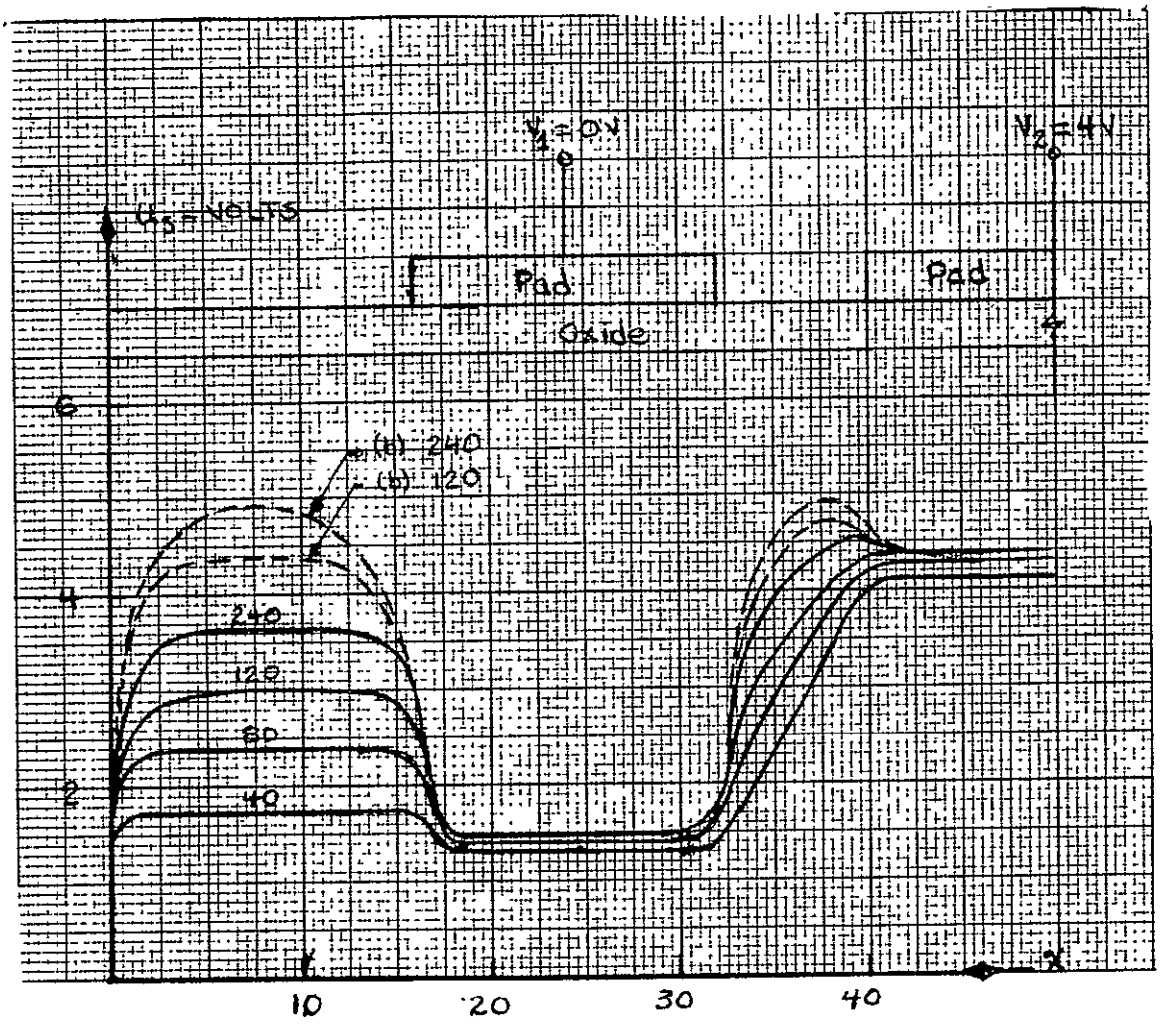
In the following we shall refer to the residual, R, which is the change in the potential at a point during an iteration. R_i is the maximum change on the interface and R_{max} is the maximum change on the entire field. As a test case we chose a configuration similar to Amelios[6] with the following parameters:



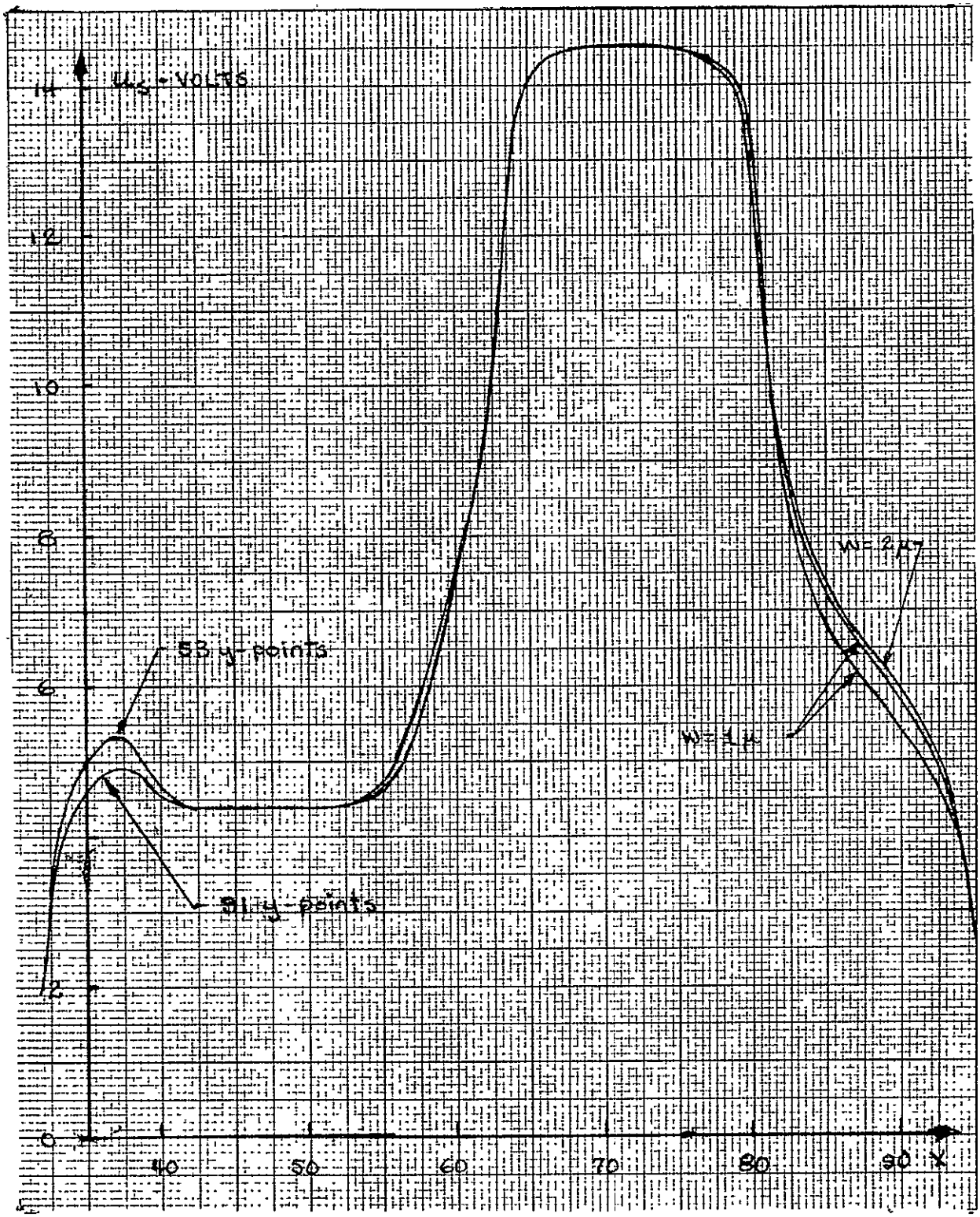
3.3



3.2 Interface Residuals vs. Iteration Number.



3.4 Surface Potential Profile for Various Number of Iteration. Label (b) indicates starting solution with oxide field equal to zero.



3.5 Profiles for Different Grid Spacing.
240 iterations.

V_1	= 0	L_G	= 8	Q_{ss}/q	= $2 \times 10^{11} cm^{-2}$	L_1	= 50
V_2	= 4	L_p	= 16	N_a	= 5×10^{14}	L_2	= 10
V_3	= 16	N	= 1μ	L_D	= .183μ	L_3	= 10
						L_4	= 10

We concluded that it would take about 240 iterations, using 193 seconds of CPU time on a UNIVAC 1106, to develop the essential features of a solution using 8736 grid points and a zero initial estimate for the potential. Starting with a better initial estimate the time is cut in half. Using a coarser grid speeds the convergence with the penalty of loss of resolution. Figure 3.6 shows the solution in the vicinity of the two electrodes with higher voltages. Reduction of the y grid from 91 lines to 53 lines shows the gap potential slightly higher but essentially the same solution with about one-half the computing time. A reduction of the x-grid from 96 to 48 lines shows essentially the same solution. This latter solution uses 2544 grid points and the CPU time is 80 seconds. The maximum y grid spacing in the substrate is 0.49μ compared with a deBye length of 0.183μ. However, the agreement of all the solutions under the low voltage electrode indicates that the space charge averaging technique is adequate.

3.4 Program Features

The program allows the operator to establish a large number of the significant parameters of a CCD structure. Geometrical features such as oxide thickness, electrode thickness and width, and gap spacing may be controlled. Other parameters such as Q_{ss}, substrate doping, shallow channel doping (treated as a surface distribution), and the electrode

voltages can be established. The number of steps through the coarser substrate grid, the oxide, through the electrodes and in the air space above is under the operator's control. The number of steps through the fine substrate grid is set in the program. These parameters are read in as input data.

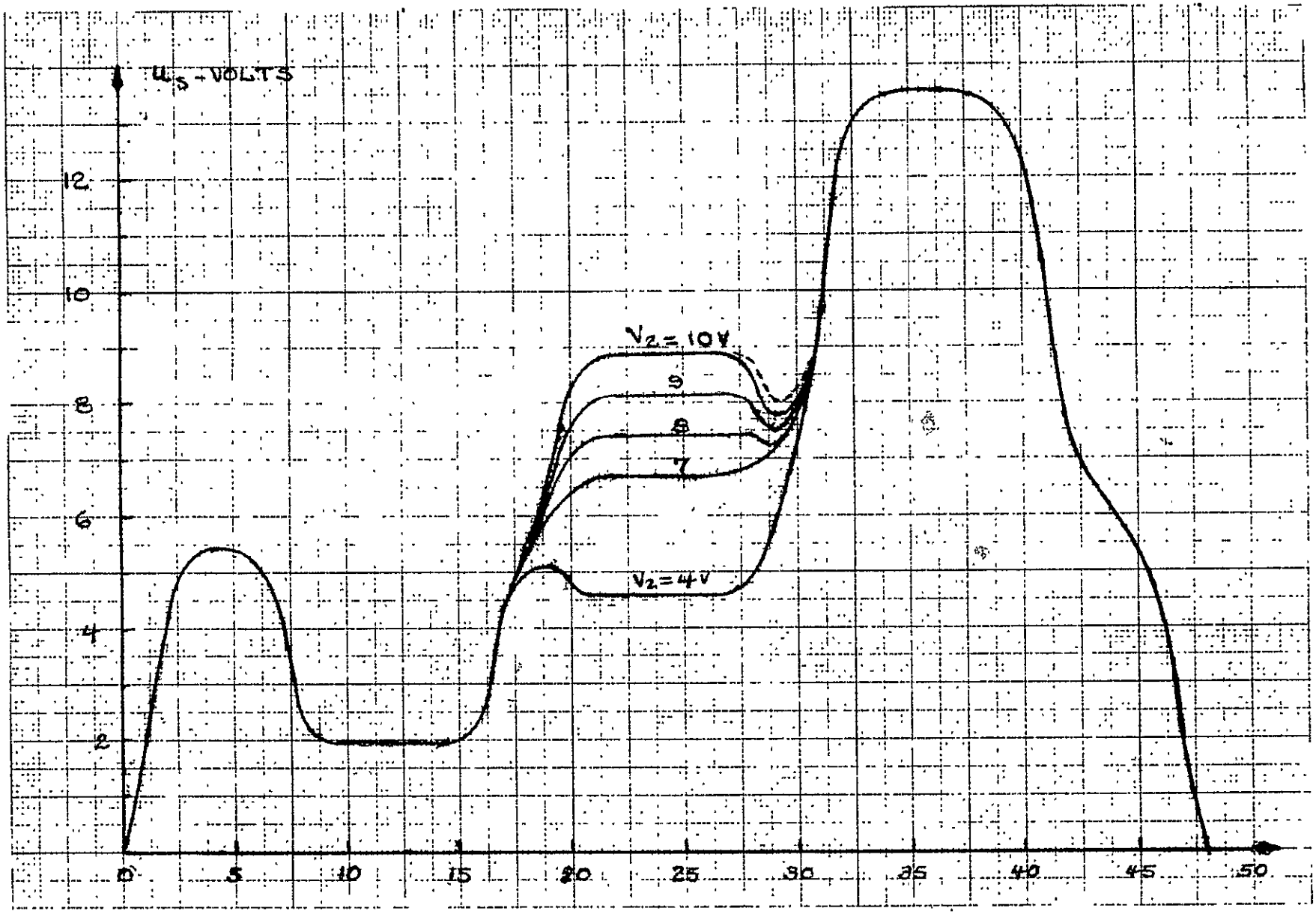
The output of the program gives the estimated maximum depletion depth, the deBye length, the y-grid values with respect to a zero origin at the interface, the indices of boundaries of discontinuity, the residuals R_i and R_{max}, and potentials along chosen lines.

The number of iterations is fixed by the parameter ITER, and the iteration numbers at which a printout of u is desired is fixed by the parameter LAP. The number of lines to be skipped is fixed by the parameter JC. These parameters are read in as data. Anyone with programming experience can easily modify these features to suit his own ideas of convenience. We believe that output of such a program should be monitored to determine the nature of convergence rather than to rely on built-in tests. Simple built-in tests would be easy to implement but may not be reliable or more complex tests may result in unnecessary costs of computing time.

Instructions on preparation of data cards for using the program are given in Appendix A.

3.5 Application of the Program

The applications of the program to 3-phase structures are obvious. For example, the potential profiles can be checked for wells and barriers as a function of gap width and channel doping. Let us consider the structure for which results were given in Figures 3.5 and 3.6 and

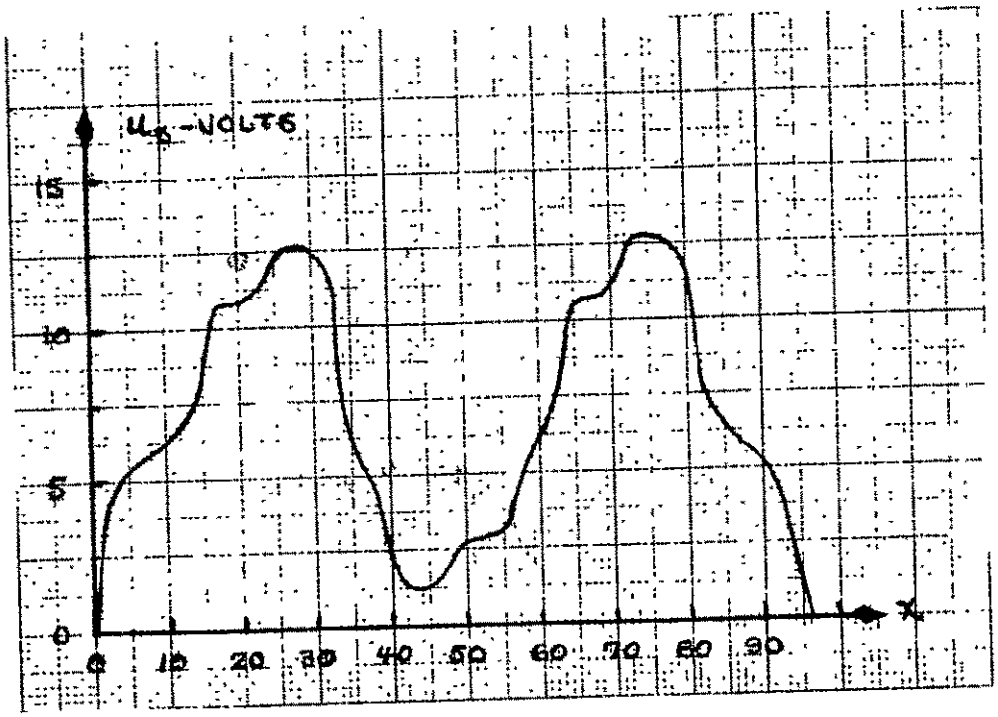


3.6 Effect of changing V_2.

assume a practical clockwave form for the transfer electrodes. Such a waveform is shown in Figure 3.7 which shows a rapidly rising leading edge and a slow trailing edge. By analyzing the potential profiles for several voltage values on electrode 2, we can find the range in which transfer can take place and estimate the fraction of a clock period for which transfer can occur. Profiles are shown in Figure 3.8. These solutions are obtained using a 2448 point grid which preserves the essential features of the solution as was illustrated in Figure 3.6. The solution for $V_2 = 4$ used 240 iterations, although inspection of the output data showed that 120 iterations gave the same answer to within 0.6%. Succeeding values for V_2 used 80 iterations each. The dotted curve shows the solution starting with $V_2 = 10$ and running 240 iterations. The entire set of data can be generated with 182 seconds of CPU time. The results show that charge can be transferred during the time V_2 is between about 5 and 7.5 volts.

The program is also applicable to the study of a 2-phase structure. figure 3.9 shows the potential profile at the interface for a structure with doping in the gap and under the left hand electrode edges such as proposed by Krambeck et. al. (Section 1, Ref. 4). The results show how that doping effects an asymmetry which allows unidirectional transfer of charge. The doping and geometric parameters were established on the basis of one-dimensional calculations, and the program verifies that the scheme will work. In this case, the experimental work at Bell Labs has proven the feasibility.

The last application considered here is for studying gate action. We give no results, since it requires modification of the program. We plan to add the modification later to be used as an option, but a



3.7 Profiles for Implanted 2-Phase Structure.

programmer can do it for himself. Suppose that a diffused junction is to the left and under electrode 1. If the junction is forward biased, the potential in that region is very near the substrate (about - .5 volts). The potential can be set to zero in that region, and the effect of varying the voltage V_1 can be studied. On the right hand side a collector junction region can be located where a positive (for n-channel) potential is specified, and the effect of V_3 in controlling the output gate can be studied. The techniques used in specifying the gate voltage and in carrying out the relaxation through the electrode region are applicable.

3.6 Determination of the Electric Field

We have not included an algorithm in the program for calculating the electric field. In the case where one wishes to estimate transit time, one must, of course, have this data. It is on this point that some criticize the numerical solution method because simple two-point numerical differentiation leads to large discontinuities in the field profile. The method for estimating the transit time must be chosen before it is clear just what data is needed; however, for the preceding cases only the x-component of the field at the interface will probably be sufficient. After a solution for U_s is determined, a high-order polynomial fit to the potential profile will allow a smooth approximation of the field at grid points.

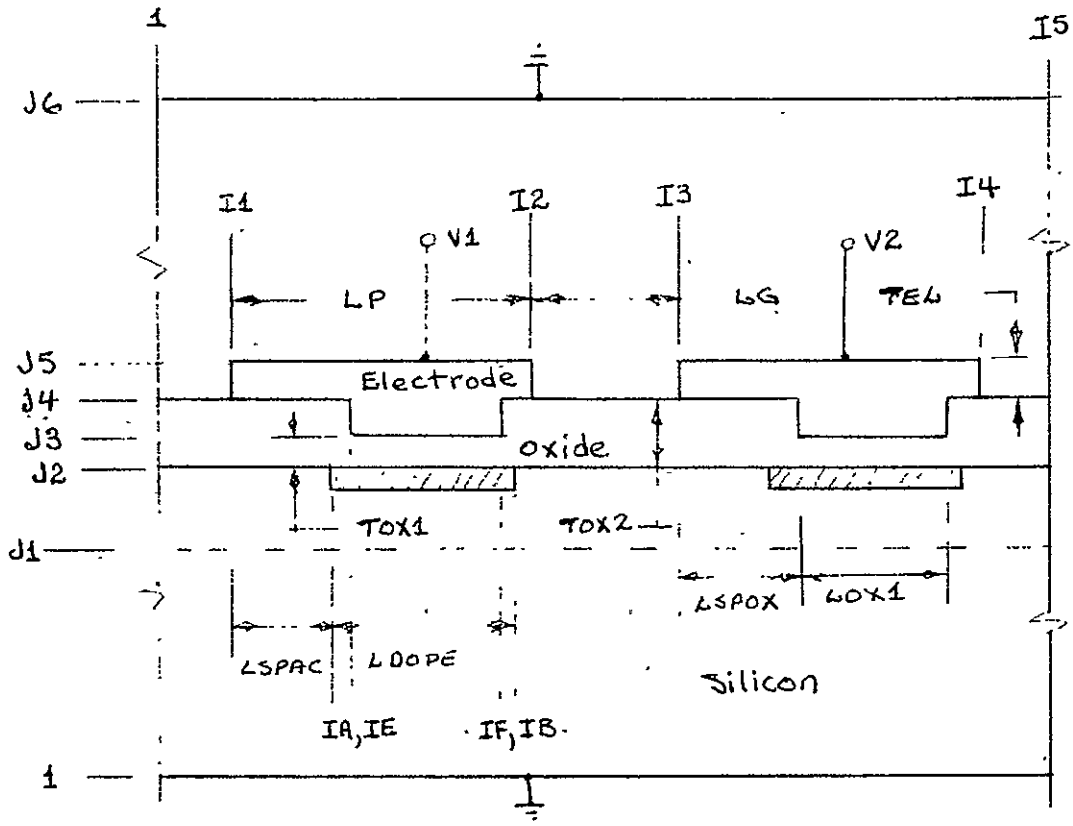
4. TWO-DIMENSIONAL ANALYSIS OF A TWO-ELECTRODE STRUCTURE

The two-electrode structure is a natural one for studying charge transfer in a 2-phase CCD. The program given in Appendix B applies the methods discussed in Section 2 to analyze the structure shown in Figure 4.1. The program has a few features which are different insofar as the programming is concerned and allows the consideration of an oxide with two thicknesses. Basically the program is the same as that in Appendix A. Periodic boundary conditions are natural for studying the inter and intra-cell transfer of charge, and these are incorporated in the program.

4.1 Program Features

The two oxide thickness feature mentioned above is a completely new and distinct feature of this program compared with the 3-electrode program. The width of the thin oxide region is controlled by the parameter LOX1. The location of the thin oxide region with respect to the left hand edge of an electrode is controlled by the parameter LSPOX. The thin and thick oxide thicknesses are TOX1 and TOX2 respectively.

In addition, the shallow doping feature is slightly different from the 3-electrode program. In the 3-electrode program the channel charge was lumped with QSS to form an effective interface surface charge. In the 2-electrode program QSS and QS(I) are separated. The doping is included in QS(I) and is read in as an effective surface charge, QP under the pads and QG in the gaps. These numbers are positive if the ionic charge is positive. Internal to the program, and beginning with line 194 of the program listing after the instruction labeled 126, is an algorithm



4.1 Two-Electrode Structure.

which determines a volume distribution coefficient CHION(J). The algorithm distributes the ions over 10 lines of the y-grid according to a Gaussian formula with a mean of YBAR and standard deviation of SIGMA. We realize that this is a simplistic procedure, especially if two types of ion are involved. However, this procedure seems to obtain solutions with essentially correct features without introducing kinks in the potential profile due to abrupt changes in QS(I). The product QS(I)*CHION(J) gives the volume space charge weight in a cell. This technique can be used to handle buried layers where the doping is of a polarity and sufficiently heavy to shift the maximum potential away from the interface. A trial run may be required to determine whether more than 10 lines are needed for the distribution. If the layer is deep compared with a deBye length, which doesn't seem likely, then shifting the desired 10 (or whatever) lines to a location beginning below the interface may be desirable. This can be done several ways in the program.

The doping QP starts LSPAC steps from the left hand electrode edge (LSPAC negative places QP to the left) and extends for a width of LDOPE steps. Making LDOPE = LP and LSPAC = 0 and QP = QG, or simply letting QP = QG = 0 and QU equal the uniform implanted layer surface density, allows treatment of a buried layer.

The 2 electrode formulation allows a finer grid for the same electrode and gap geometry, and the program has a feature which allows the relaxation procedure to bypass the lower lines in the substrate where changes are extremely slow. As changes occur which advance the depletion layer, the relaxation procedure then start a line lower, etc. All of these factors allow the program to run with a higher resolution grid and shorter time when compared with the 3-electrode program.

4.2 Application of the Program

We have chosen an example which we believe illustrates the manner in which two-dimensional analysis programs are useful as design aids. Creative thinking of a semi-quantitative nature concerning CCD's will probably rely on one-dimensional models. The two-dimensional analysis can check the validity of the conclusions arrived at from a one-dimensional consideration.

The structure shown in Figure 4.2 appears to have some promise for 2-phase CCD application. The two-oxide thicknesses allow an asymmetry necessary for unidirectional transfer. The electrode voltage will pull the surface potential higher under the thin oxide. The surface charge in the gap region, from either QSS or uniform implantation, pulls the surface potential high enough to preclude a barrier in the gap. Implantation through the thin oxide allows a sufficient surface charge to maintain a high potential on the right side of the interface even when the electrode voltage is low.

We start with the MIS equations:

$$\psi_s = V_a + V_b - (2V_aV_b + V_b^2)^{1/2} \tag{4.1a}$$

$$V_a = V_G + \frac{Q_s}{C_{ox}} \tag{4.1b}$$

$$V_b = \frac{qN\epsilon_s}{C_{ox}^2} \tag{4.1c}$$

$$\psi_g = \frac{Q_g^2}{2qN\epsilon_s} \tag{4.2}$$

where in (4.2) it is assumed that the oxide field is zero. Now we assume that $Q_{s2} = Q_g$, $Q_{s1} = \gamma Q_g$, and $C_{ox1} = \eta\, C_{ox2}$. Next we define

the parameters $\beta = qN\epsilon_s/C_{ox2}Q_g$ and $\alpha = V_G/\psi_g$. We then divide ψ_s by ψ_g and write expressions for the normalized potential in each region:

$$\psi_{N1} = \frac{\psi_{s1}}{\psi_g} = \alpha + \frac{2\gamma}{\eta}\beta + \frac{2\beta^2}{\eta^2} - \frac{2\beta}{\eta}\left(\alpha + \frac{2\gamma\beta}{\eta} + \frac{\beta^2}{\eta^2}\right)^{1/2} \tag{4.3}$$

$$\psi_{N2} = \frac{\psi_{s2}}{\psi_g} = \alpha + 2\beta + 2\beta^2 - 2\beta(\alpha + 2\beta + \beta^2)^{1/2} \tag{4.4}$$

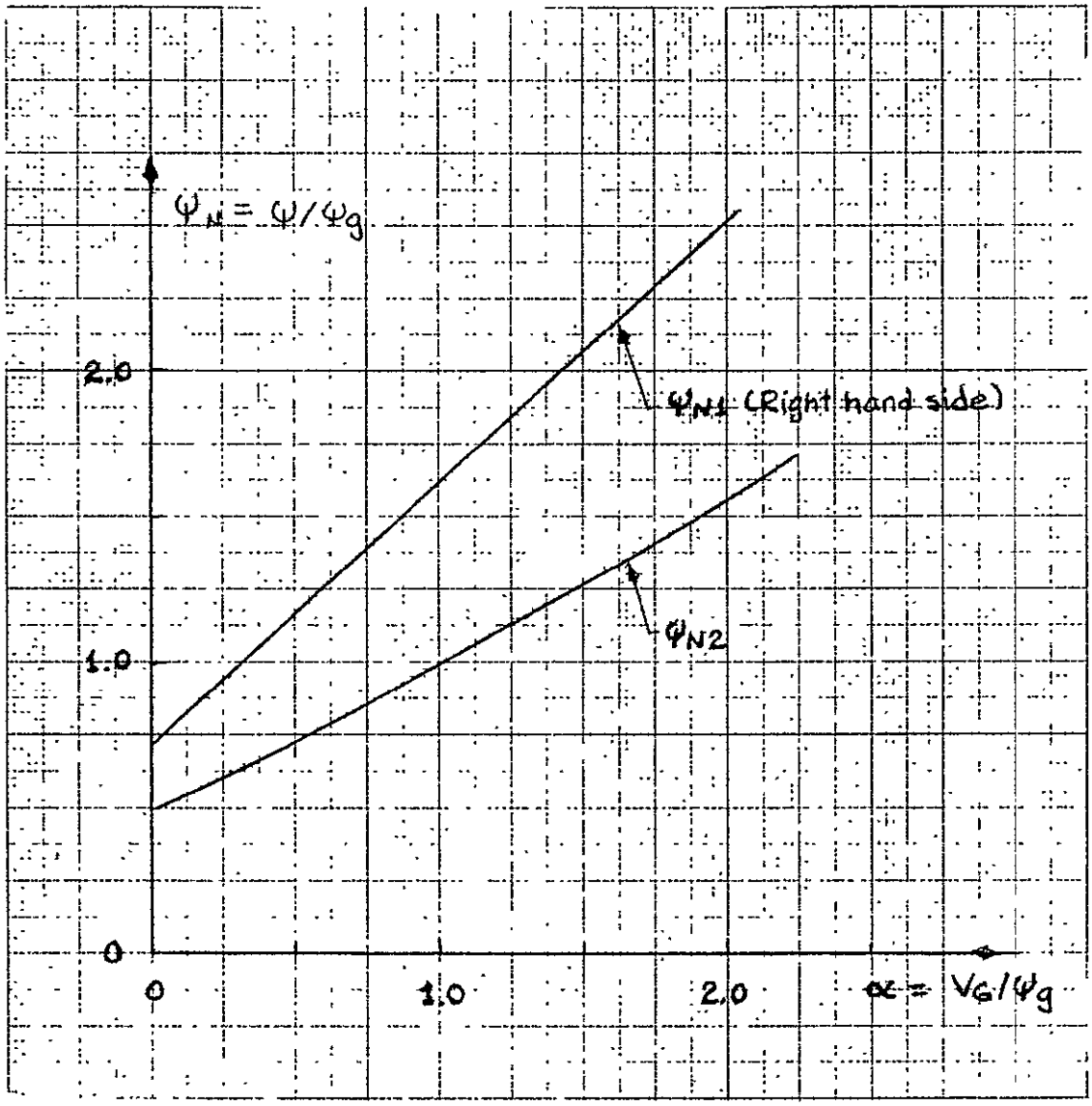
Let us choose the oxide thicknesses to be 0.1μ and 0.5μ , thin enough and thick enough for selective ion implantation. Now with zero electrode voltage we wish to make $\psi_{N2} < \psi_{N1} < \psi_g$ so that minority carriers are shifted always to the right hand edge. Setting $\alpha = 0$ and solving for β from (4.4) and γ from (4.3), we obtain:

$$\beta = \frac{\psi_{N2}(1 \pm \sqrt{\psi_{N2}})}{2(1 - \psi_{N2})} \tag{4.5}$$

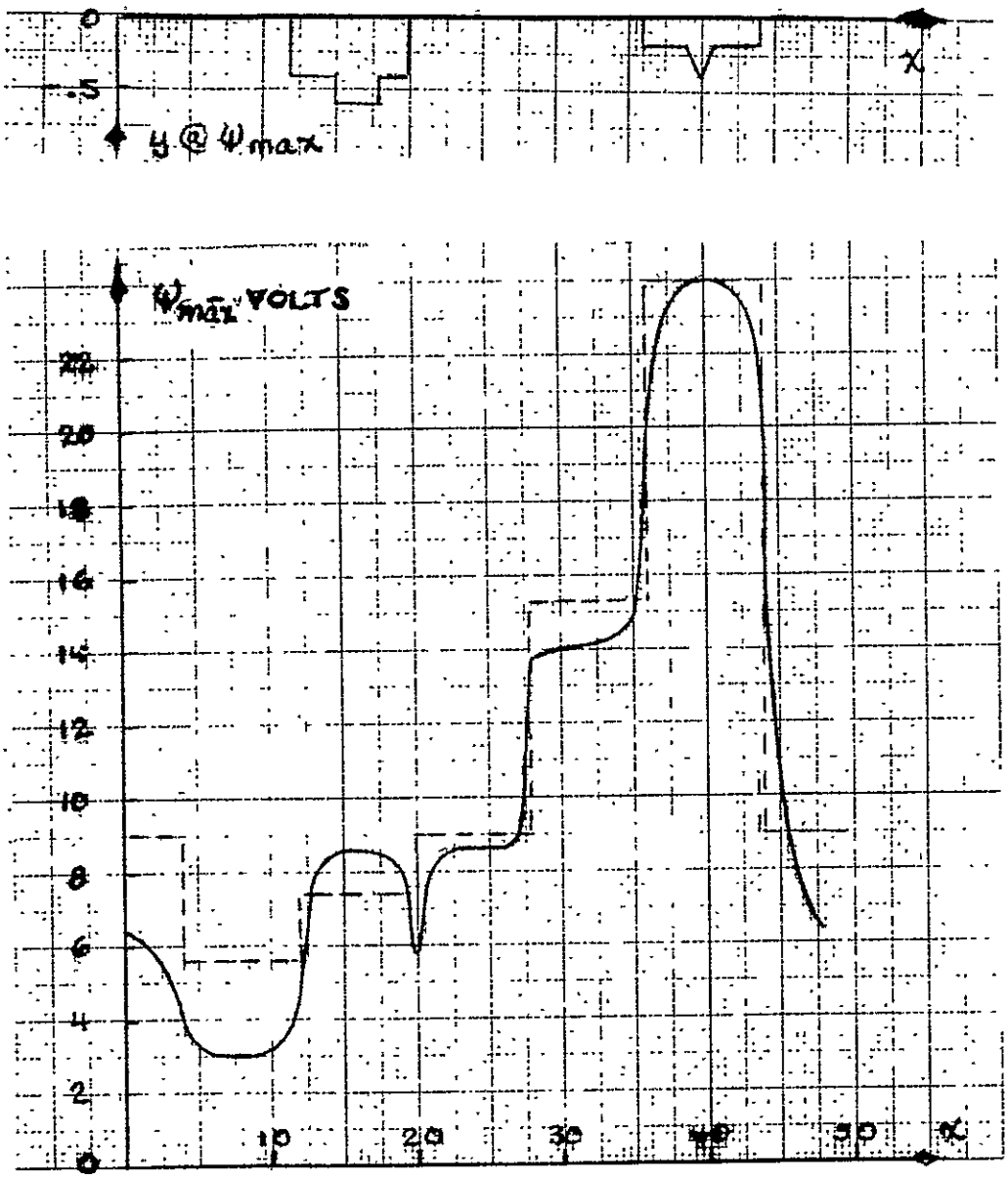
$$\gamma = \frac{\eta\psi_{N1}}{2\beta} \pm \sqrt{\psi_{N1}} \tag{4.6}$$

We choose the positive signs in equations (4.5) and (4.6) and let $\psi_{N2} = 1/2$, $\psi_{N1} = 3/4$. This gives $\beta = 0.853$ and $\gamma = 3.066$ so that $Q_g/q = 6.7 \times 10^{11}\text{cm}^{-2}$, $\psi_g = 8.6\text{V}$, and $Q_p/q = 2.05 \times 10^{12}\text{cm}^{-2}$ with a substrate doping of $N_a = 3.8 \times 10^{16}\text{cm}^{-3}$ and $n = 5$.

Figure 4.2 shows the normalized surface potential vs. the normalized transfer electrode voltage. Choosing $V_{g2} = 20\text{V}$ gives $\alpha = 2.33$, and this should work well for obtaining a transfer. In Figure 4.3 the maximum potential profile is shown along with the location of the maximum potential. In the more heavily doped regions the maximum potential occurs below the interface as is shown in Figure 4.3. This accounts in part for



4.2 Normalized Potentials on Right and Left Hand Sides of Electrode Versus Normalized Gate Voltage.

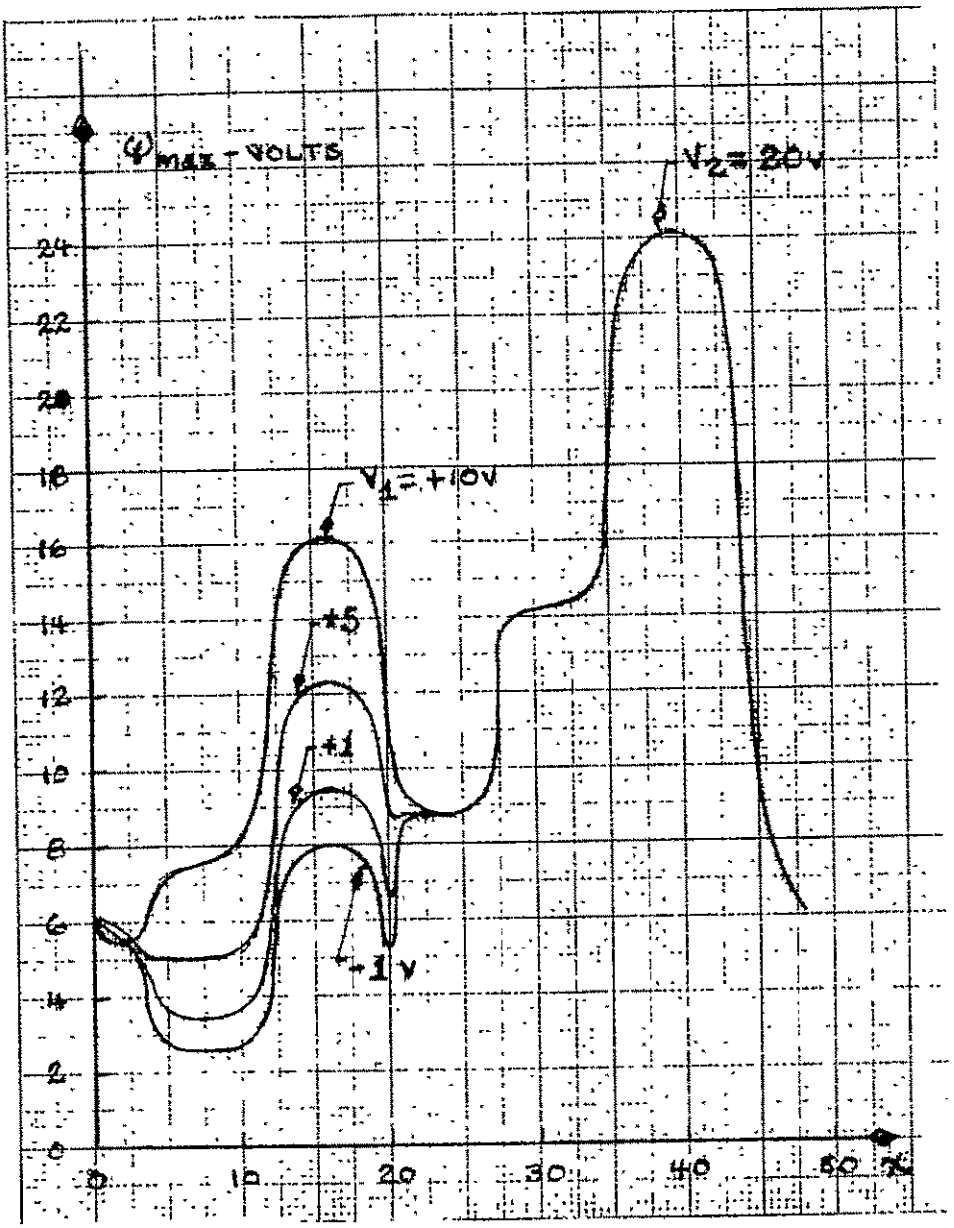


4.3 Maximum Substrate Potential Profile.
x in microns.

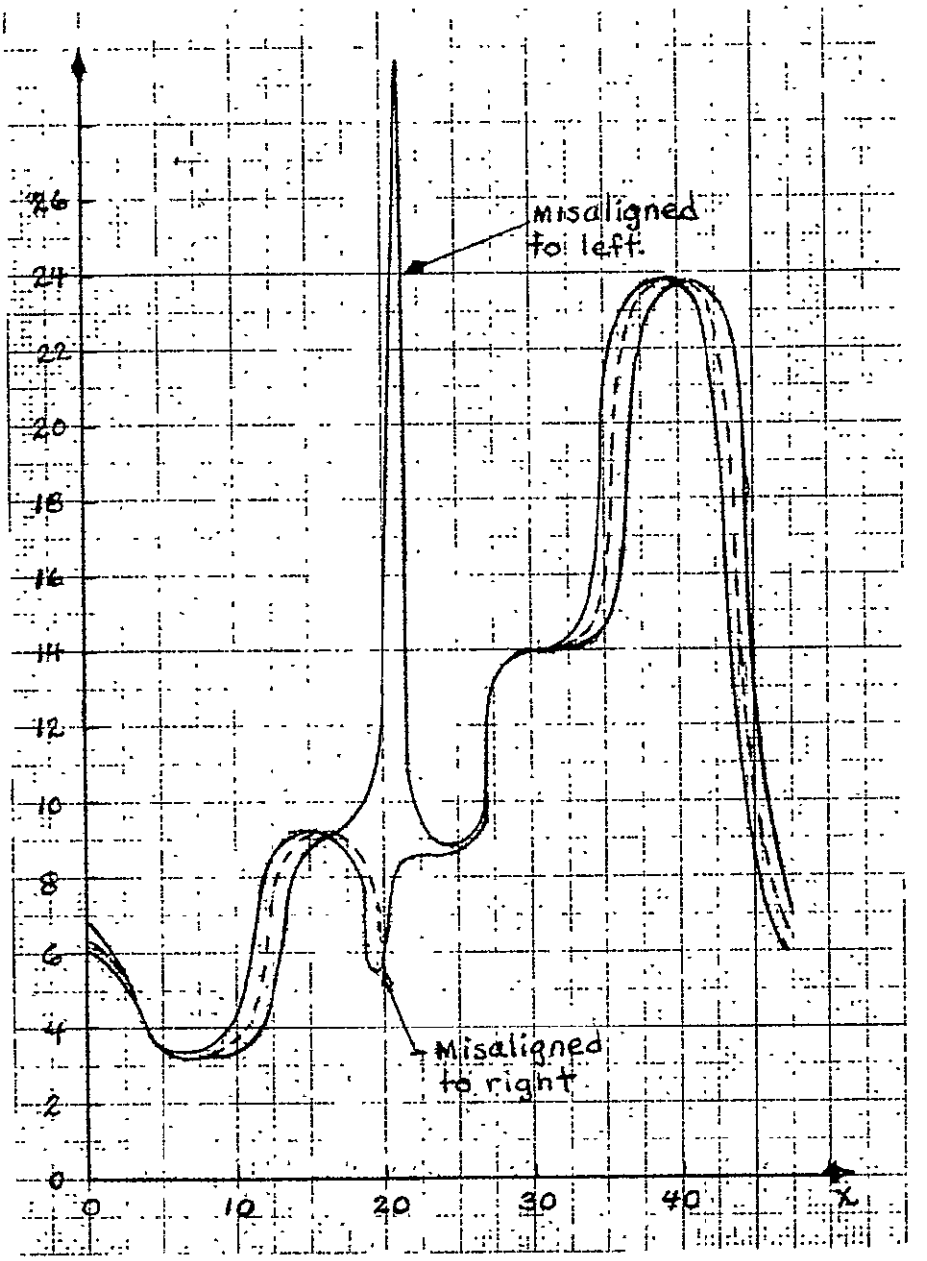
the rise of the potential above the predicted value from the one-dimensional approximation shown in dotted lines. A gaussian distribution of the implanted charge is assumed. It is observed that a potential barrier occurs at the right hand edge of the low voltage electrode for $V_{G1} = 0$. Therefore, charge would be trapped under this electrode. One observes that the potential maximum is located deeper underneath the low voltage electrode than under the high; therefore, the ratio of the trapped charged to the amount which can be stored under the high voltage electrode is somewhat lower than it first appears. Most of the charge which can be stored under the high voltage electrode will be on the right-hand side with the higher oxide capacitance. Neglecting the differences in location of the potential maximum the ratio of the trapped charge to maximum stored with electrode voltages of 0 and 20V is:

$$r_T \cong \frac{2.3\ C_{ox1}}{5.2\ C_{ox2} + 15.2\ C_{ox1}} \cong 14\%$$

Figure 4.4 shows the effect of misalignment of the electrodes with respect to the oxide. Misalignment to the right accentuates the barrier, and misalignment to the left introduces a well for trapping charge. The absence of a peak in the profile at the right hand edge of the 20V electrode was unexpected and caused us to do some intensive checking of the program but we found no errors. Finally, Figure 4.5 shows the profile for a sequence of values for V_{G1} indicating the possibilities for charge transfer for practical clock waveforms on the transfer electrodes. In conclusion, even with $\pm$ 1μ misalignment the trapped charge is of a tolerable magnitude for CCD operation.



4.4 Profiles for Various Values of V_1.



4.5 Effect of Misalignment of Electrodes.

4.3 Possible Modifications

Some may have objections to the using the smaller increments beneath the interface. This feature can be modified by rewriting the subroutine YSPAC. The feature can be deactivated by removing the card sequence; H0 = 3.0 *TOX1/L3 to J2 = J1 + L2 and setting J2 = J1.

The distribution of implanted charge can be modified by allowing it to go further into the grid, i.e., increasing the limit LL = 10 and dimensioning CHION( ) suitably. The function used can be changed by defining parameters other than YBAR and SIGMA or changing their values. The most flexible approach is to substitute a subroutine function say FIMPL(A,B, ···,Z) for the gaussian function used. However, a suitable function can be incorporated in the main program also.

4.4 Use of the Program

The program uses approximately 20,000 words or 80,000 BYTES of storage. Of this 11,000 words are used for storage of the field points. This can be reduced by a factor of 4 for many cases by redimensioning the arrays for a coarser grid. The run time for 240 iterations and a 3504 point field is 240 seconds of CPU time.

The charge entered as QG, QP, AND QS will be distributed according to the same function as the program is now written. QG will be located in the gaps between the electrodes. QP can be placed anywhere under or to the side of an electrode. QU is uniform all across the surface. QSS is treated as a pure surface charge uniformly distributed.

The thin oxide region can be located as desired. The left hand edge is specified and the width of the region specified.

Read in data for the program is as follows:

1. READ(S,1) JA,JB,JC,MAXU,IRES
   1 FORMAT(SI10)
   JA: lowest line of potentials to be printed out.
   JB: highest line of potentials to be printed out.
   JC: steps between lines printed out.
   Internally, program adjusts JA≥1 , JB≤J6 , such that the line for J=J2 (interface) is printed.
   MAXU: set to integer greater than zero if the maximum substrate potential profile is desired.
   IRES: set to integer greater than zero if a printout of the residuals after each iteration is desired.
   (Recommended for a first time through until confidence in convergence is established.)

2. READ(S,2)TOX1, TOX2,TEL,W,HFAC
   2 FORMAT(5F10.3)
   TOX1: thin oxide thickness in microns.
   TOX2: thick oxide thickness in microns.
   TEL: electrode thickness in microns.
   W: width of grid cell in microns.
   HFAC: (HFAC > 1.0) multiplies estimated depletion depth to set zero potential boundary in substrate.
   Default value is HFAC = 2.0.

3. READ(5,4)QSS,CSUB,QG,QP,QU
   4 FORMAT(5E10.3)
   QSS: surface state charge, cm^{-2} (i.e. QSS/q)
   CSUB: substrate doping, cm^{-3}.
   QG: gap doping, cm^{-2}.
   QP: under electrode doping, cm^{-2}
   QU: uniform doping, cm^{-2}.

4. READ(5,6)V1,V2,ITER,LAP
   6 FORMAT(2F10.3,2I10)
   V1: left hand electrode voltage, volts.
   V2: right hand electrode voltage, volts.
   ITER: total number of iterations. (Try 120-240 for start)
   LAP: printout control, printout occurs when iteration parameter LOOP/LAP = Integer

5. READ(5,18)LP,LG,LOOPE,LSPAC,LOX1,LSPOX
   LP: Pad width in units of w.
   LG: gap width in units of w.
   LDODE: width of underpad doping in units of w.
   LSPAC: location of underpad doping from left hand electrode edge in units of w, positive to the right.
   LOX1: width of thin oxide region in units of w.
   LSPOX: spacing of thin oxide region with respect to left hand electrode edge in units of w, positive to the right.

6. READ(5,408)OM1,OM2,OM3,OM4,OM5
408 FORMAT(5F10.3)
These are the relaxation parameters for the 5 regions. After early experimentation we used: (1.8,1.8,1.5,1.5,1.5).
The user may start with these and do his own experimentation.

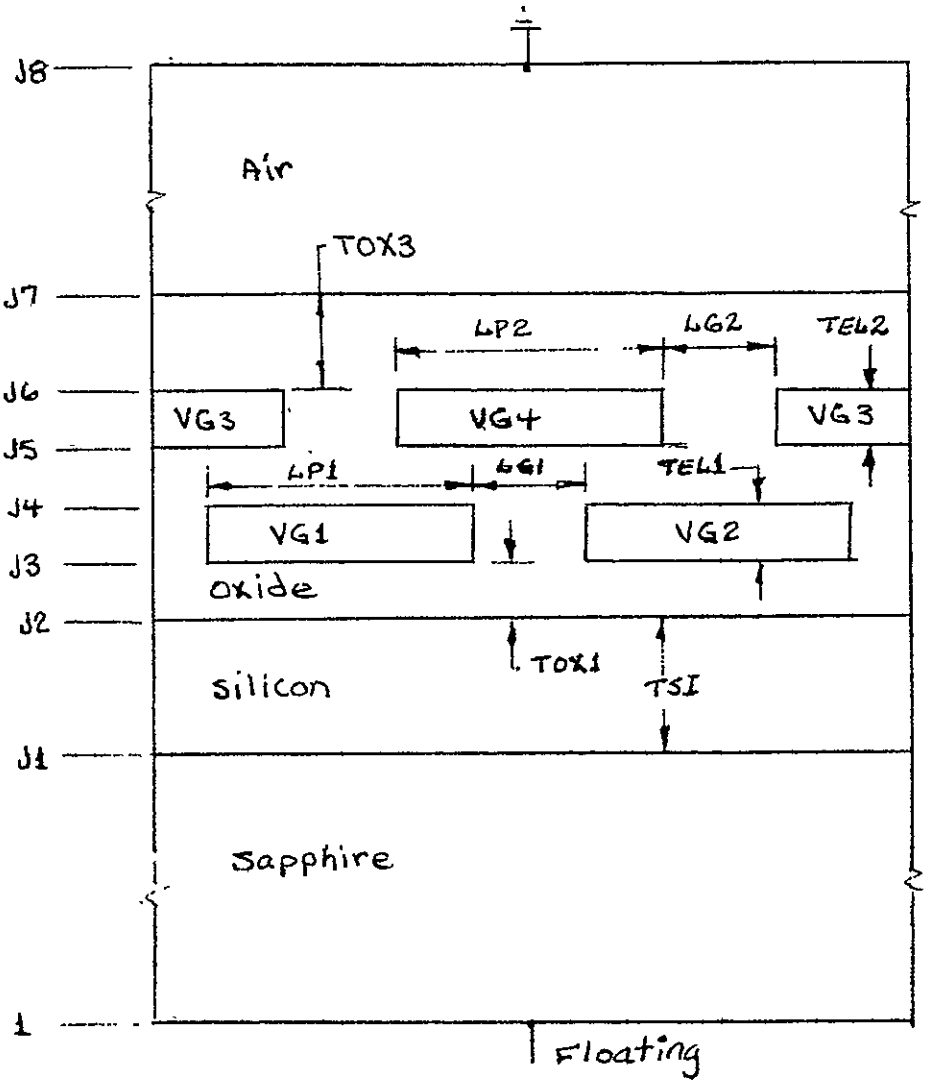
7. READ(5,6) V1,V2,ITER,LAP
Repeat for as many subsequent values as required.
The solution builds on the last solution obtained.
If V1 and V2 are not changed more than 1V
ITER = 50 should suffice.

8. BLANK CARD.
Computation terminates after test on a blank card.

5. TWO-DIMENSIONAL ANALYSIS OF A FOUR-ELECTRODE STRUCTURE

This structure, illustrated in Figure 5.1, seems to be popular for CCD design because it provides complete electrostatic shielding of the channel. Originally, it was recognized as a possible solution to the problem of electrostatic barriers which may occur in the gaps; however, it was later recognized that shielding precludes the build-up of a static surface charge which influences the interface potential in an unpredictable manner.

Although we have seen no reports of operation of CCD's constructed in silicon-on-sapphire (SOS), we believe that this type of design is under consideration. Imaging devices using a 4-electrode structure would appear to be quite attractive as an application of silicon on transparent sapphire. SOS has not been attractive for bipolar devices because of the relatively low life-times due to surface recombination. Apparently lack of availability of the material or economic factors have held back application in the MOS area. We did a rough sensitivity check using the surface state density data of Elliot and Anderson[1] and assuming a 2.5μ sec lifetime and that the thin silicon layer would be depleted. For a one micron layer, visual inspection reveals that most of the incident light is absorbed; therefore, we conclude that after a reflection from a conducting boundary essentially all incident radiation would be absorbed. We obtained a sensitivity of approximately $4mw/cm^2$ assuming a quantum efficiency of unity. After making several conversions of units which we hope were correct, we found that the sensitivity of a "sensitive" phottransistor currently available is approximately $2mw/cm^2$. This latter figure no doubt includes the effects of a lens, etc., but is still useful.



$$J_n = J_{n-1} + L_n$$

5.1 Four-Electrode Structure. Silicon is assumed to be depleted by an appropriate arrangement not revealed by two-dimensional geometry used for periodic boundary conditions.

We assume that others have checked the sensitivity and found it to be tolerable.

The program which we describe in this section can be used to analyze a 4-electrode SOS structure. However, it can also be used to analyze a 4-electrode CCD structure on a silicon substrate.

5.1 Program Features

The program provides for a sapphire substrate. Since the substrate is relatively thick compared with the epitaxial silicon layer, the y-grid spacing in the substrate is exponential. Treating the sapphire as infinite in extent and applying LaPlace's equation we estimate that the field is attenuated by $e^{-2\pi}$ at a depth equal to the width of one cell in a periodic structure. Periodic boundary conditions are used for the potential variation along the x-direction. Exponential y-grid spacing would correspond roughly to equi-potential points along an x-cut through the grid. The substrate charge gives rise to a "d.c." field component, the value of which depends upon the thickness of the sapphire substrate and the boundary condition of the surface. It seems probable that the sapphire would be greater than 250μ thick and that a transparent, grounded conductor would be placed on the surface to eliminate static charge. With this thickness the d.c. field component would be small; therefore, we set the field equal to zero at a distance of one cell depth into the sapphire. For the silicon-substrate option, the boundary conditions in the substrate are similar to the previous programs.

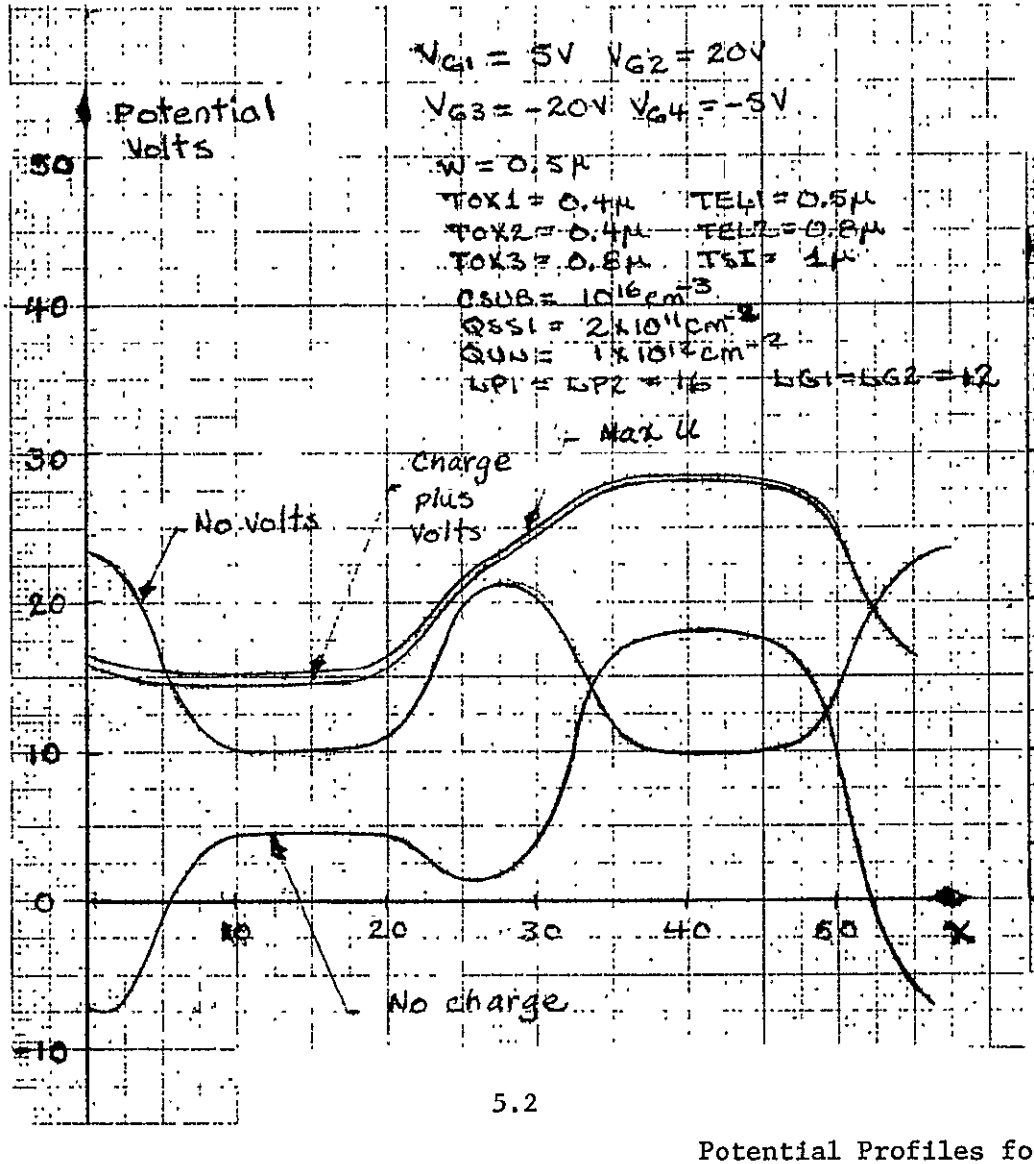
The analysis assumes that the silicon is depleted; therefore, the results are meaningful only if depletion can be maintained. It is of course conceivable to have a silicon film thick enough so that depletion

is not complete. Such a structure may be in fact required to allow depletion for the full length of the channel, but we do not know the answer at this time. If this is true, then the sapphire substrate feature is superfluous; however, the program can still handle the problem. Since total absorption is possible within a thin, completely depleted film, it seems desirable to obtain this situation if possible. The program allows the dimensions of the electrodes, the doping, oxide thickness, electrode thickness and electrode voltages to be controlled. The relative positions of the electrodes is fixed; however, this seems to be no serious limitation. The number of iterations is controlled on the same data card with the electrode voltages so that subsequent runs with perturbations of the electrode voltages are possible.

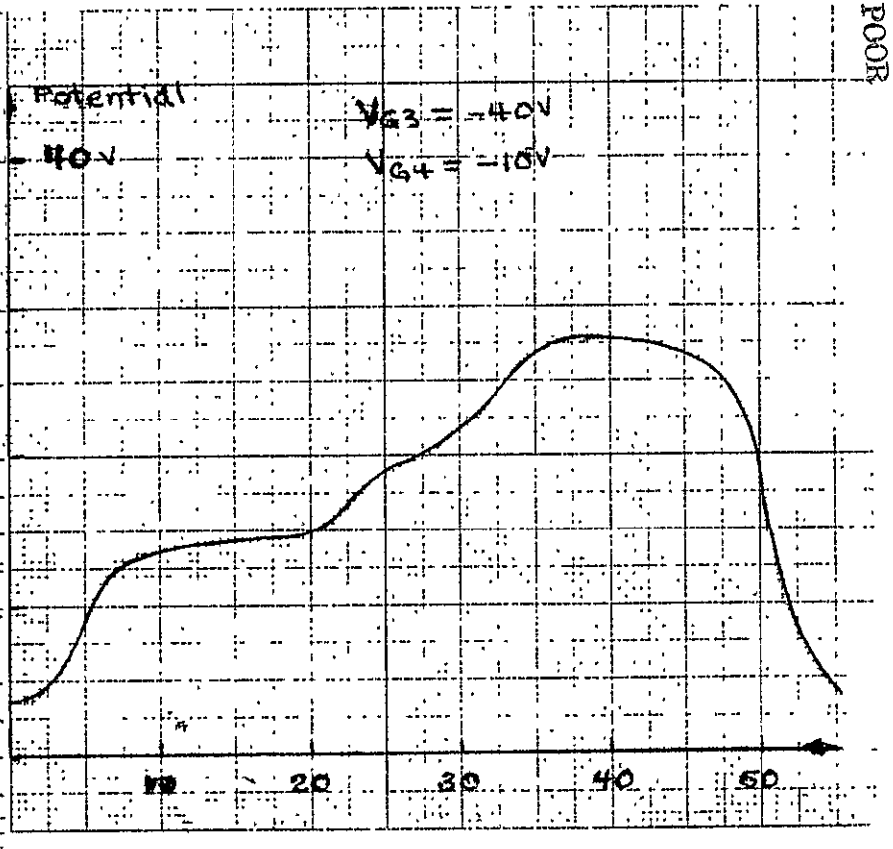
Spacing is uniform in each of six regions and exponential in the sapphire and airspace regions. The exponent will usually be smaller for the silicon substrate, since the grid usually will span a smaller distance. In this case, the maximum error which may occur due to round-off of the space-charge is:

$$\frac{\delta u_s}{u_s} = \frac{.2\ \alpha^{L1}(\ -1)}{L2(\alpha-1) + \alpha^{L1-1} - 1}$$

If one is concerned with error other than at the interface, the above relationship is not valid. We feel that the grid spacing for the silicon substrate needs further consideration, since it is definitely compromised for simplicity and compatibility with the case for a sapphire substrate.

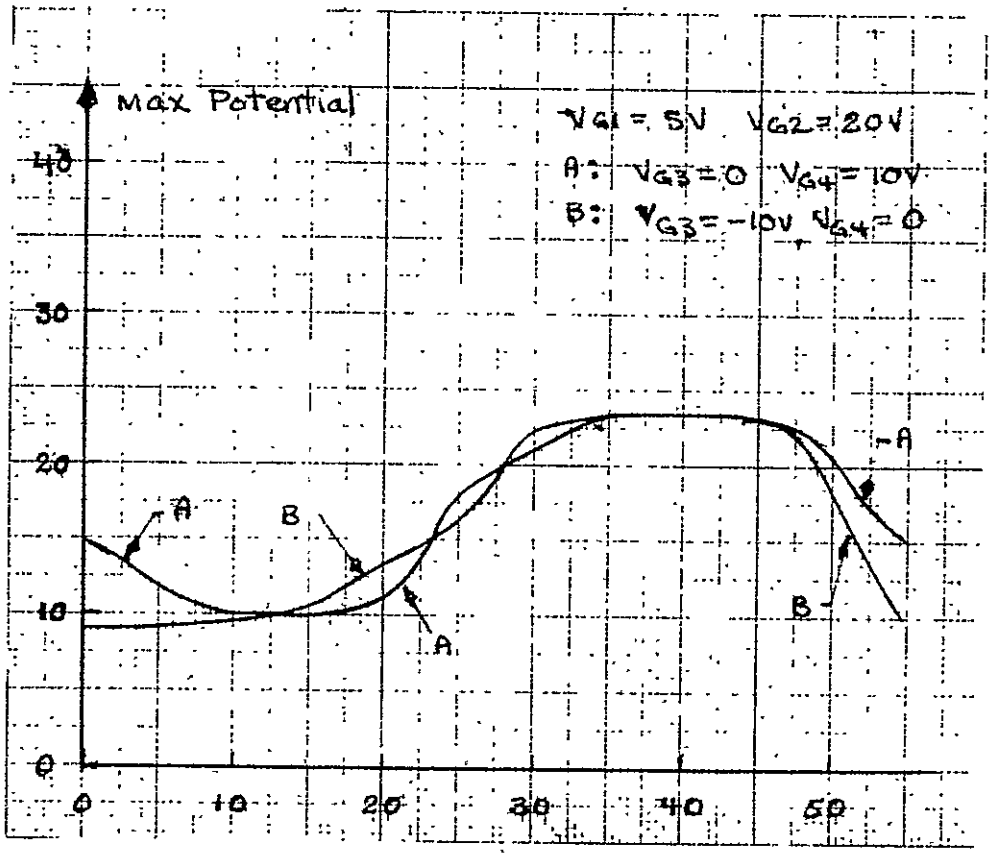


5.2



5.3

Potential Profiles for SOS Structure



5.4 Potential Profile, Four-Electrode, Silicon-Substrate Structure.

5.2 Application for the Program

Figure 5.2 shows results obtained in applying the program to an SOS structure. Curves are shown for zero space charge, for zero pad volts, and for the composite. Since the problem is linear, the two individual source curves should add to produce the composite. It can be seen that they do. One notes that the peaks of the potential curves for zero volts are not equal as they should be. It was suspected and confirmed that a programming error resulted in shortening the upper left electrode and shifting of the upper electrodes to the left. This gave complete coverage for the center electrode but not the left hand and right hand gaps. The error was corrected. The results, however, do not give the asymmetry required for transferring charge undirectionally.

Figure 5.3 shows the potential profile for electrode voltages which give the asymmetry required. The values required would not lead to convenient waveform generation; however, it is not our purpose here to propose a practical design.

Figure 5.4 shows the potential profiles obtained applying the program to a silicon substrate. TSI, QUN, SIGMA, and YBAR are chosen to obtain an N-layer 1 microns thick with a doping of $3 \times 10^{15} cm^{-3}$. The P-substrate is doped with $10^{15} cm^{-3}$. The resultant profile in A would not allow undirectional charge transfer. Some items of interest for this curve are as follows. The residual dropped from 4.52V to 1mV in 240 iterations requiring 149 seconds CPU time. The depletion depth occurred at $y = -5.25\mu$ and $h = 0.48\mu$ giving a maximum roundoff error of approximately 10%. The field contains 4047 grid points.

The curve labeled "B" shows sufficient asymetry to make charge transfer to the right possible. The maximum potential occurs at a

distance from 0 to 0.4μ below the Si-SiO_2 interface. Unfortunately, under the pad where charge would be transferred to, the maximum occurs on the surface. However, these results are given to illustrate the program capacilities and not to suggest a practical design.

5.3 Use of Program

The program is approximately the same size and takes approximately the same running time as the 3-electrode program discussed in Section 4. Convergence is obtained within 240 iterations to within 3% or better with the residuals typically dropping from approximately 5 volts to 10mV. Such a run requires 158 seconds with 4047 grid points in the field.

The dimensions of the arrays must be checked for compatibility with the desired number of grid points. The dimensions in the listed program allow 100 x 100 points. The listing is given in Appendix C.

Input data cards are in the sequence given below:

	DATA	FORMAT
1.	LP1,LG1,LP2,LG2,ITYPE,MAXO ITYPE=0, sapphire substrate; ITYPE = 1, silicon. MAXU=1 for printout of u_{max}, otherwise MAXU=0.	6I10
2.	JA,JB,JC JA: lower line printed out; JB: upperline; JC: number of lines skipped.	3I10
3.	L1,L2,L3,L4	4I10
4.	L5,L6,L7,L8	4I10
5.	TOX1,TEL1,TOX2,TEL2	4F10.3
6.	TOX3,TSI,W	4F10.3
7.	QSS1,QSS2,QUN,CSUB QSS1: Si-SiO_2 interface surface state density, cm^{-2}. QSS2: Si-Sapphire interface surface state density, cm^{-2}. QUN: Uniform implanted density, cm^{-2}.	4E10.3

	DATA	FORMAT
8.	VG1, VG2,VG3,VG4,1TER,LAP (see Section 4 for more information.)	4F10.3,ZI10
9.	OM1,OM2,OM3,OM4,YBAR,SIGMA Try omega value between 1.5 and 1.8 Subroutine DISFAC uses YBAR and SIGMA as the usual parameters of a gaussian function in coordinate variable y to specify implanted doping.	6F10.3

10.- Repeat card (8) for as many values as desired.

(Last) Blank card terminate program.

References

1. A. B. M. Elliot and J. C. Anderson, Solid State Electronics, Vol. 15, pp. 531-545, 1972.

6. CONCLUSION

We have described three programs which can be used to obtain an electrostatic analysis of CCD structures. These programs cover a broad variety of structures which may be of interest. When the computed profiles are such that uni-directional charge transfer is possible, then such profiles may be considered to be approximately those which would exist in a structure operating in an ideal mode with a small amount of "signal" charge in any given cell. The profiles also serve as a base for estimating the amount of charge corresponding to a "full well".

Other work which we have done on CCD's during the past year includes dynamic analysis of charge transport. Our work has been confined to one-dimensional models, and we have studied the so-called "flux-corrected" method for solving the transport equations. We are not ready to report on this work at this time. The emphasis which has been given to buried layer devices and the observations which we have made from electrostatic analyses makes it clear to us that accurate models of the transport equation must also be two-dimensional. If one does not use two-dimensional models, then it seems that the techniques used by Kosonoeky and Carnes and Amelio (references in Section 1) are adequate for estimates of the transit time. It should be noted that a two-dimensional analysis will require at least twice as much data storage as the electrostatic analysis. Computing time will be at least doubled and probably increased well beyond that. However, we intend to pursue this problem further.

APPENDICES

The following listings are of programs written in FORTRAN V. All programs are approximately the same size. Program 2, Appendix B, requires 20,000 words or 80,000 BYTES of storage. The field points require approximately 11,000 words. Without changing the arrays, all programs handle a grid of 100 x 100 points. (Appendix B program 100 x 110). Runs will require up to 240 iterations per solution with about 4 minutes on a UNIVAC 1106, or equivalent, for one solution using 10,000 points. Reduction of the number of field points will reduce the run time proportionally.

To use, supply run control cards, with appropriate control cards also separating the main and subprograms, and prepare data cards describing structure according to formats given. Suggested trial values of relaxation parameter are between 1.5 and 1.8 with 1.7 a good value to start with.

APPENDIX A

THREE-ELECTRODE PROGRAM

See section 3, Figure 3.1 for diagram of structure.

Data cards:

	DATA	FORMAT
1.	JA,JB,JC JA: Lowest line of potential array printed. JB: Highest line of potential array printed. JC: Spacing between lines. Program recompute JA and JB to obtain printout of line J2, the Si-SiO_2 interface.	3I10
2.	TOX,TEL,W,CDEBY,CDEPL Default values of CDEBY and CDEPL are 2. See text for discussion of optimizing these values. Program will run well on default values.	5F10.3
3.	QSS,CSUB,QG,QP See listing and text for further information.	4E10.3
4.	V1,V2,V3,ITER,LAP Try first runs with ITER = 240, LAP = 40. This will give approximately 50 pages of output data including listing. After inspection for convergence, both ITER and LAP may be reduced.	3F10.3,2I10
5.	L1,L3,L4,L5 See Figure 3.1 text. For example, L1 = J1-1 , L2 = J2-J1, etc.	4I10
6.	LP,LG,LDOPE,LSPAC See listing and text for further information	4I10
7.	Repeat card 5 for as many solutions as desired.	
8.	Last data card is blank to stop computation.	

```
X.DECK,,MINE
B69     01/28-11:47:17

000   @RUN    CCD2,EE0017U,JIM,,/50
000   @ASG,T   TEMP,F2
000   @FLT,LIB TEMP.PCH
000   C      ********************************************************
000   C      ELECTROSTATIC ANALYSIS OF CCD STRUCTURE
000   C      DIMENSION ARRAYS, DEFINE COMMON VARIABLES
000   C       H IS THE GRID SPACING NORMAL TO THE INTERFACE
000   C       W   '   '   '   PARALLEL WITH THE INTERFACE
000   C       U IS THE ELECTROSTATIC POTENTIAL WRT THE SUBSTRATE BULK
000   C       DU IS THE RESIDUAL
000   C      ********************************************************
000          COMMON U(100,100),DU(100),H(100),FO,L2,ALPHA,IMAX,JMAX,EA,EB,
000         *A,B,C,G,W,VT,I,J,DUMAX
000          DIMENSION QS(100)
000          VT=0.0259
000   C*********************************************************
000   C      READ LINE PRINTOUT CONTROL  PARAMETERS
000   C*********************************************************
000          READ(5,1) JA,JB,JC
000     1    FORMAT(3I10)
000   C      ********************************************************
000   C       READ DIMENSIONS OF REGION FOR ANALYSIS, MICRONS
000   C      ********************************************************
000   C      ********************************************************
000   C       TOX= OXIDE THICKNESS
000   C       TEL= ELECTRODE THICKNESS
000          READ(5,2) TOX,TEL,W,CDEBY,CDEPL
000       2  FORMAT(5F10.3)
000   C       QSS= SURFACE STATE CHARGE,CM-2
000   C       CSUB= SUBSTRATE DOPING,CM-3
000   C      QG= GAP DOPING,CM-2,POSITIVE IF CHARGE POSITIVE
000   C      QP= UNDERPAD DOPING, ' '   '''    '''
000   C      ********************************************************
000          READ(5,4)QSS,CSUB,QG,QP
000     4    FORMAT(4E10.3)
000   C    'SIGN' IS USED TO PRECLUDE SPACE CHARGE INSTABILITY IN RELAXATION
000   C     IN SUBSTRATE. IF 'U' HAS WRONG SIGN, 'U' IS SET TO ZERO.
000          SIGN=-1.0
000          IF(CSUB.GT.0.0)  SIGN = 1.0
000   C      ********************************************************
000   C      READ ELECTRODE VOLTAGES,NUMBER OF ITERATIONS,AND LOOP PRINTOUT
000   C      ********************************************************
000          READ(5,6) V1,V2,V3,ITER,LAP
000       6  FORMAT(3F10.3,2I10)
000   C      ********************************************************
000   C       COMPUTE CHARGE DENSITY PARAMETERS
000   C      ********************************************************
000          Q=1.6E-19
000          EO=8.85E-14
000          VSS=Q*QSS/EO*1.E-4
000          VSUB=-Q*CSUB/EO*1.E-8
000          CON=2.*11.7*EO/(Q*CSUB)
000   C      ********************************************************
000   C       ESTIMATE DEPLETION DEPTH
```

```
000   C      ESTIMATE SURFACE POTENTIAL
000   C     ***************************************************************
000          ABV1=ABS(V1)
000          ABV2=ABS(V2)
000          ABV3=ABS(V3)
000          VG=V1
000          IF(ABV2.GT.ABV1) VG=V2
000          IF(ABV3.GT.ABV2) VG=V3
000          CO=3.9*8.85E-14/(1.E-4*TOX)
000          VA=VG+QSS*Q/CO
000          VB=Q*CSUB/CO*11.7*EO/CO
000          PSI= VA+VB-SQRT(2.*VA*VB+VB**2)
000          XDS=2.*11.7*EO/Q*PSI/CSUB
000          XD=SQRT(ABS(XDS))*1.E4
000   C     ***************************************************************
000   C      FIND THE EXTRINSIC DEBYE LENGTH
000   C     ***************************************************************
000          DL=VT*11.7*EO/Q/CSUB
000          EDL=SQRT(DL)*1.E4
000   C     ***************************************************************
000   C      WRITE DEPLETION DEPTH AND DEBYE LENGTH
000   C     ***************************************************************
000          WRITE(6,300) XD,EDL
000      300 FORMAT('1',10X,'DEPLETION DEPTH =',F10.3,5X,'DEBYE LENGTH=',F10.3)
000   C     ***************************************************************
000   C     ***************************************************************
000   C      DETERMINE NORMAL CONTROL INDICES
000   C      AND SET THE Y-GRID SPACING
000   C      L1, REGION OF UNIFORM SPACING IN SEMICONDUCTOR
000   C      L2,'    ' EXPONENTIAL  ' , '
000   C      L3, '   '   UNIFORM '   ' OXIDE
000   C      L4, '   ' ,'     '   THROUGH ELECTRODES
000   C      L5, '   '   EXPONENTIAL '    '   IN AIRSPACE
000   C     ***************************************************************
000          READ(5,302)  L1,L3,L4,L5
000      302 FORMAT(4I10)
000          J1=L1+1
000          K1=L1
000          IF(CDEPL.LT.1.0) CDEPL=2.0
000          DO 8 J=1,K1
000          H(J)=CDEPL*XD/L1
000      8   CONTINUE
000          HO=3.*TOX/L3
000          IF(HO.GT.EDL) HO=EDL
000          IF(CDEBY.LT.2.) CDEBY=2.
000          YO=CDEBY*HO
000          FO=YO/HO
000          CALL YSPAC
000          J2=J1+L2
000          K2=J2-1
000          DO 10 JJ=1,L2
000          J=J2-JJ
000          H(J)= HO*ALPHA**JJ
000      10  CONTINUE
000          J3=J2+L3
000          K3=J3-1
000          DO 12 J=J2,K3
```

```
000          H(J)=TOX/L3
000       12 CONTINUE
000          J4=J3+L4
000          K4=J4-1
000          DO 14 J=J3,K4
000          H(J)=TEL/L4
000       14 CONTINUE
000          J5=J4+L5
000          K5=J5-1
000          DO 16 J=J4,K5
000          JJ=J-J4
000          H(J)=(TEL/L4)*(2.**JJ)
000       16 CONTINUE
000     C    ************************************************************
000     C    PRINT OUT THE Y-COORDINATE VALUES AND THECONTROL INDICES
000     C    ************************************************************
000          WRITE(6,17)
000       17 FORMAT(/,10X,'THE Y-COORDINATE VALUES ARE:'/)
000          Y=0.
000          DO 125 J=J2,K5
000          Y=Y+H(J)
000          WRITE(6,127) Y
000       125 CONTINUE
000          Y=0.
000          DO 129 LL=1,K2
000          J=J2-LL
000          Y=Y-H(J)
000          WRITE (6,127) Y
000       129 CONTINUE
000       127 FORMAT(F20.6)
000          WRITE(6,131) J1,J2,J3,J4,J5
000       131 FORMAT(//,10X,'J-VALUES ARE:',5I10//)
000     C    COMPUTE JA,JB VALUES TO OBTAIN INTERFACE PRINTOUT
000          MT=(J2-JA)/JC
000          JA=J2-MT*JC
000          IF(JB.GT.J5) JB=J5
000     C    ************************************************************
000     C     DETERMINE LATERAL CONTROL INDICES
000     C    LP AND LG ARE THE NUMBER OF STEPS ACROSS THE PAD AND GAP.
000     C    THEN COMPUTE THE SURFACE CHARGE DISTRIBUTION
000     C    ************************************************************
000          READ(5,18) LP,LG,LDOPE,LSPAC
000       18 FORMAT(4I10)
000          I1=LP+1
000          I2=I1+LP
000          I3=I2+LG
000          I4=I3+LP
000          I5=I4+LG
000          I6=I5+LP
000          I7=I6+LP
000          IA=(I2+I3)/2
000          IB=(I4+I5)/2
000          IC=I1+LSPAC
000          ID=IC+LDOPE
000          IE=I3+LSPAC
000          IF=IE+LDOPE
000          IG=I5+LSPAC
```

```
000          IH=IG+LDOPE
000          DO 333 I=2,I7
000          QS(I)=QSS+QG*(F(1,I1,I)+F(I2,I3,I)+F(I4,I5,I)+F(I6,I7,I))
000         *+QP*(F(IC,ID,I)+F(IE,IF,I)+F(IG,IH,I))
000          QS(I1)=QS(I1)-QG/2.
000      333 CONTINUE
000          QS(I2)=QS(I2)-QG/2.
000          QS(I3)=QS(I3)-QG/2.
000          QS(I4)=QS(I4)-QG/2.
000          QS(I5)=QS(I5)-QG/2.
000          QS(I6)=QS(I6)-QG/2.
000          QS(IC)=QS(IC)-QP/2.
000          QS(ID)=QS(ID)-QP/2.
000          QS(IE)=QS(IE)-QP/2.
000          QS(IF)=QS(IF)-QP/2.
000          QS(IG)=QS(IG)-QP/2.
000          QS(IH)=QS(IH)-QP/2.
000    C     ************************************************************
000    C      SET THE ELECTRODE POTENTIALS
000    C     ************************************************************
000          DO 28 J=J3,J4
000          DO 26 I=I1,I6
000          U(I,J)=V1*F(I1,I2,I)+V2*F(I3,I4,I)+V3*F(I5,I6,I)
000       26 CONTINUE
000       28 CONTINUE
000    C     ************************************************************
000    C    SET VALUES BETWEEN ELECTRODES ON AIR-OXIDE INTREFACE
000    C     ************************************************************
000          J=J3
000          DO 240 I=2,I1
000          U(I,J)= U(1,J)+(I-1)*(U(I1,J)-U(1,J))/(I1-1)
000      240 CONTINUE
000          DO 242 I=I2,I3
000          U(I,J)=U(I2,J)+(I-I2)*(U(I3,J)-U(I2,J))/(I3-I2)
000      242 CONTINUE
000          DO 244 I=I4,I5
000          U(I,J)=U(I4,J)+(I-I4)*(U(I5,J)-U(I4,J))/(I5-I4)
000      244 CONTINUE
000          DO 246 I=I6,I7
000          U(I,J)=U(I6,J)+(I-I6)*(U(I7,J)-U(I6,J))/(I7-I6)
000      246 CONTINUE
000    C     ************************************************************
000    C    INITIALIZE POTENTIAL DISTRIBUTION IN THE SEMICONDUCTOR AND
000    C     OXIDE USING THE ONE DIMENSIONAL DEPLETION LAYER ESTIMATE.
000    C     VB DEFINED ABOVE
000    C     ************************************************************
000          DO 406 I=2,I7
000          J=J2
000          VS=U(I,J3)
000          VAA=Q*QS(I)/CO
000          VA=VS+VAA
000          IF(I.GT.1.AND.I.LT.I1) GO TO 398
000          IF(I.GT.I2.AND.I.LT.I3) GO TO 398
000          IF(I.GT.I4.AND.I.LT.I5) GO TO 398
000          IF(I.GT.I6.AND.I.LT.I7) GO TO 398
000          VINT=VA+VB-SQRT(2.*VA*VB+VB**2)
000          GO TO 399
```

```
000     398  VINT=Q*(QS(I)**2)/(2.*11.7*EO*CSUB)
000     399  CONTINUE
000          XDS=CON*VINT
000          XD=SQRT(ABS(XDS))
000          Y=0.
000     400  J=J-1
000          Y=Y+H(J)
000          YN=1.E-4*Y/XD
000          IF(YN.GE.1.)    GO TO 402
000          U(I,J)=VINT*(1.-YN)**2
000          GO TO 400
000     402  J=K2
000          Y=0.
000     404  J=J+1
000          Y=Y+H(J)
000          YN=Y/TOX
000          IF(YN.GE.1.) GO TO 406
000          U(I,J)=VINT+(VS-VINT)*YN
000          GO TO 404
000     406  CONTINUE
000     C*************************************************************
000     C    WRITE OUT THE STRUCTURE PARAMETERS
000     C*************************************************************
000          WRITE(6,345) TOX,TEL,W,V1,V2,V3,LP,LG,LDOPE,LSPAC,QSS,QG,QP,CSUB
000      345 FORMAT(/,10X,'TOX,TEL,W=',3F10.3/10X,'V1,V2,V3=',3F10.3/
000         *10X,'LP,LG,LDOPE,LSPAC=',4I10/10X'QSS,QG,QP,CSUB=',4E15.3/)
000     C    ***************************************************
000     C    READ RELAXATION PARAMETER VALUES
000     C    ***************************************************
000          READ(5,408) OM1,OM2,OM3,OM4,OM5
000      408 FORMAT(5F10.3)
000          KT=1
000          JLO=J1/2
000          JHI=J4+1
000     C    ***************************************************
000     C     START THE RELAXATION PROCEDURE STARTING AT THE LOWEST ROW
000     C     AND WORKING ACROSS TO THE RIGHT TO THE TOP ROW
000     C    ***************************************************
000          LOOP=1
000      800 CONTINUE
000          DUMAX=0.
000          DO 40 J=JLO,K2
000          EA=11.7
000          EB=11.7
000          A=EA*W/H(J-1)
000          B=(EA*H(J-1)+EB*H(J))/(2.*W)
000          G=EB*W/H(J)
000          C=A+2.*B+G
000          OMEGA=OM1
000          DO 38 I=2,I7
000          IF(U(I,J+1).EQ.0.0) GO TO 33
000       30 TEST=ABS(U(I,J-1)/VT)
000          IF(TEST.GT.4) GO TO 31
000          ITEST=1
000          QIJ=VSUB*AVERO(ITEST)
000          GO TO 32
000       31 QIJ=VSUB*W*(H(J)+H(J-1))/2.0
```

```
000      32  UOLD=U(I,J)
000          UTIL=(A*U(I,J-1)+B*U(I-1,J)+B*U(I+1,J)+G*U(I,J+1)+QIJ)/C
000          U(I,J)=(1.-OMEGA)*UOLD+OMEGA*UTIL
000          US=SIGN*U(I,J)
000          IF(US.LT.0.0) U(I,J)=0.0
000          DU(I)=U(I,J)-UOLD
000          GO TO 36
000      33  IF(U(I+1,J).EQ.0.0) GO TO 34
000          GO TO 30
000      34  IF(U(I-1,J).EQ.0.0) GO TO 38
000      36  CALL MAXOF
000      38  CONTINUE
000      40  CONTINUE
000    C     ************************************************************
000    C      RELAX THE SILICON,SILICON-DIOXIDE INTERFACE
000    C     ************************************************************
000          J=J2
000          EA=11.7
000          EB=3.9
000          A=EA*W/H(J-1)
000          B=(EA*H(J-1)+EB*H(J))/(2.*W)
000          G=EB*W/H(J)
000          C=A+2.*B+G
000          OMEGA=OM2
000          DO 48 I=2,I7
000          QSA=(QS(I+1)+QS(I-1))/2.
000          TEST=ABS(U(I,J-1)/VT)
000          IF(TEST.GT.4) GO TO 42
000          ITEST=3
000          QIJ=VSUB*AVERO(ITEST)+Q*QSA/EO*1.E-4
000          GO TO 44
000      42  QIJ=VSUB*H(J-1)*W/2.+Q*QSA/EO*1.E-4*W
000      44  UOLD=U(I,J)
000          UTIL=(A*U(I,J-1)+B*U(I-1,J)+B*U(I+1,J)+G*U(I,J+1)+QIJ)/C
000          U(I,J)=(1.-OMEGA)*UOLD+OMEGA*UTIL
000          US=SIGN*U(I,J)
000          IF(US.LT.0.0) U(I,J)=0.0
000          DU(I)=U(I,J)-UOLD
000          CALL MAXOF
000      48  CONTINUE
000          DMAX=0.0
000          J=J2
000          DO 696 I=2,I7
000          IF(ABS(DU(I)).GT.DMAX)IM=I
000     696  IF(ABS(DU(I)).GT.DMAX)DMAX=ABS(DU(I))
000          WRITE(6,697)DMAX,IM
000     697  FORMAT(2X,'DU=',F5.3,5X,'I=',I3)
000    C     ************************************************************
000    C      RELAX THE OXIDE REGION
000    C     ************************************************************
000          JJ=J2+1
000          DO 60 J=JJ,K3
000          EA=3.9
000          EB=3.9
000          A=EA*W/H(J-1)
000          B=(EA*H(J-1)+EB*H(J))/(2.*W)
000          G=EB*W/H(J)
```

```
000           C=A+2.*B+G
000           OMEGA=OM3
000           DO 58 I=2,I7
000           QIJ=0.0
000           UOLD=U(I,J)
000           UTIL=(A*U(I,J-1)+B*U(I-1,J)+B*U(I+1,J)+G*U(I,J+1)+QIJ)/C
000           U(I,J)=(1.-OMEGA)*UOLD+OMEGA*UTIL
000           DU(I)=U(I,J)-UOLD
000           CALL MAXOF
000        58 CONTINUE
000        60 CONTINUE
000     C     ************************************************************
000     C      RELAX THE OXIDE-AIR-ELECTRODE INTERFACE
000     C     ************************************************************
000           J=J3
000           EA=3.9
000           EB=1.0
000           A=EA*W/H(J-1)
000           B=(EA*H(J-1)+EB*H(J))/(2.*W)
000           G=EB*W/H(J)
000           C=A+2.*B+G
000           DO 68 I=2,I7
000           IF(I.GE.I1.AND.I.LE.I2) GO TO 68
000           IF(I.GE.I3.AND.I.LE.I4) GO TO 68
000           IF(I.GE.I5.AND.I.LE.I6) GO TO 68
000           QIJ=0.
000           OMEGA=OM4
000           UOLD=U(I,J)
000           UTIL=(A*U(I,J-1)+B*U(I-1,J)+B*U(I+1,J)+G*U(I,J+1)+QIJ)/C
000           U(I,J)=(1.-OMEGA)*UOLD+OMEGA*UTIL
000           DU(I)=U(I,J)-UOLD
000           CALL MAXOF
000        68 CONTINUE
000     C     ************************************************************
000     C      RELAX THE ELECTRODE-AIRSPACE REGION
000     C     ************************************************************
000           JJ=J3+1
000           DO 80 J=JJ,J4
000           EA=1.
000           EB=1.
000           A=EA*W/H(J-1)
000           B=(EA*H(J-1)+EB*H(J))/(2.*W)
000           G=EB*W/H(J)
000           C=A+2.*B+G
000           OMEGA=OM5
000           DO 78 I=2,I7
000           IF(I.GE.I3.AND.I.LE.I4) GO TO 78
000           IF(I.GE.I5.AND.I.LE.I6) GO TO 78
000           IF(I.GE.I1.AND.I.LE.I2) GO TO 78
000           QIJ=0.
000           UOLD=U(I,J)
000           UTIL=(A*U(I,J-1)+B*U(I-1,J)+B*U(I+1,J)+G*U(I,J+1)+QIJ)/C
000           U(I,J)=(1.-OMEGA)*UOLD+OMEGA*UTIL
000           DU(I)=U(I,J)-UOLD
000           CALL MAXOF
000        78 CONTINUE
000        80 CONTINUE
```

```
000   C     ***************************************************************
000   C      RELAX THE AIR-SPACE REGION ABOVE THE ELECTRODES
000   C     ***************************************************************
000         JJ=J4+1
000         DO 90 J=JJ,JHI
000         EA=1.
000         EB=1.
000         A=EA*W/H(J-1)
000         B=(EA*H(J-1)+EB*H(J))/(2.*W)
000         G=EB*W/H(J)
000         C=A+2.*B+G
000         OMEGA=OM5
000         DO 88 I=2,I7
000         QIJ=0.
000         IF(U(I,J-1).EQ.0.) GO TO 84
000      82 CONTINUE
000         UOLD=U(I,J)
000         UTIL=(A*U(I,J-1)+B*U(I-1,J)+B*U(I+1,J)+G*U(I,J+1)+QIJ)/C
000         U(I,J)=(1.-OMEGA)*UOLD+OMEGA*UTIL
000         DU(I)=U(I,J)-UOLD
000         CALL MAXOF
000         GO TO 88
000      84 IF(U(I+1,J).EQ.0.) GO TO 86
000         GO TO 82
000      86 IF(U(I-1,J).EQ.0.) GO TO 88
000         GO TO 82
000      88 CONTINUE
000      90 CONTINUE
000         JLO=JLO-1
000         IF(JLO.LT.2) JLO=2
000         JHI=JHI+1
000         IF(JHI.GT.K5) JHI=K5
000   C     ***************************************************************
000   C     OUTPUT CONTROL AND ITERATION CONTROL FOLLOWS
000   C     THIS ITERATION CONTROL CAN BE REPLACED BY A CONDITIONAL
000   C     CONTROL ON EITHER DU OR DUMAX.
000   C     ***************************************************************
000         LOOP=LOOP+1
000         LWRIT=LOOP/LAP
000         IF(LWRIT.EQ.KT) GO TO 881
000     207 CONTINUE
000         IF(LOOP.LT.ITER) GO TO 800
000   C*************************************************************************
000   C     THE FOLLOWING READ MAY BE USED FOR FINDING NEW POTENTIALS
000   C     AFTER APPLYING SMALL PERTURBATIONS TO THE ELECTRODE VOLTAGES
000   C*************************************************************************
000         READ(5,6) V1,V2,V3,ITER,LAP
000         IF(ITER.EQ.0)  STOP
000         DO 883 J=J3,J4
000         DO 882 I=I1,I6
000         U(I,J)=V1*F(I1,I2,I)+V2*F(I3,I4,I)+V3*F(I5,I6,I)
000        *+(1.-F(I1,I2,I)-F(I3,I4,I)-F(I5,I6,I))*U(I,J)
000     882 CONTINUE
000     883 CONTINUE
000         LOOP=1
000         KT=1
000         GO TO 800
```

```
000    881  CONTINUE
000         WRITE(6,212) DUMAX,IMAX,JMAX
000     212 FORMAT(30X,'DUMAX=',F10.3,5X,'IMAX=',I4,5X,'JMAX=',I4)
000         DO 205 J=JA,JB,JC
000         WRITE(6,208) J
000    208  FORMAT(10X,'J=',I3)
000         WRITE(6,206) (U(I,J), I=1,IA)
000         WRITE(6,206) (U(I,J), I=IA,IB)
000         WRITE(6,206) (U(I,J), I=IB,I7)
000    206  FORMAT(10F10.2)
000    205  CONTINUE
000         KT=KT+1
000         GO TO 207
000         END
000         FUNCTION F(II,JJ,KK)
000         F=0.0
000         IF(KK.GE.II.AND.KK.LE.JJ) F=1.0
000         RETURN
000         END
000         SUBROUTINE YSPAC
000         COMMON U(100,100),DU(100),H(100),FO,L2,ALPHA,IMAX,JMAX,EA,EB,
000        *A,B,C,G,W,VT,I,J,DUMAX
000         ALPHA=1.25
000         L2=ALOG(0.25*FO+1.0)/ALOG(ALPHA)
000     2   F1=(ALPHA**L2-1.)/(ALPHA-1.)
000         TRY=ABS(F1/FO)
000         IF(TRY.LT.1.005.AND.TRY.GT.0.995) GO TO 4
000         F=F1-FO
000         LL=L2-1
000         F3=L2*(ALPHA**LL)/(ALPHA-1.)
000         F4=(ALPHA**L2-1.)/((ALPHA-1.)**2)
000         FP=F3-F4
000         ALPHA=ALPHA-F/FP
000         GO TO 2
000       4 CONTINUE
000         RETURN
000         END
000         SUBROUTINE AVERO(ITEST)
000         COMMON U(100,100),DU(100),H(100),FO,L2,ALPHA,IMAX,JMAX,EA,EB,
000        *A,B,C,G,W,VT,I,J,DUMAX
000         S=0.0
000         U1=ABS(U(I,J)+U(I,J-1))
000         IF(U1.GT.0.0) S=0.5*H(J-1)
000         IF(ITEST.GT.2) GO TO 4
000         U2=ABS(U(I,J)+U(I,J+1))
000         IF(U2.GT.0.0) S=S+0.5*H(J)
000       4 AVERO=S*W
000         RETURN
000         END
000         SUBROUTINE MAXOF
000         COMMON U(100,100),DU(100),H(100),FO,L2,ALPHA,IMAX,JMAX,EA,EB,
000        *A,B,C,G,W,VT,I,J,DUMAX
000         DOLD=ABS(DUMAX)
000         DNEW=ABS(DU(I))
000         IF(DNEW.GT.DOLD)  GO TO 2
000         GO TO 4
000       2 DUMAX=DU(I)
```

```
000          IMAX=I
000          JMAX=J
000      4   RETURN
000          END
000    @XQT
000                5          40          5
000       0.5          0.8          2.0
000       2.00E+11   5.00E+14
000       0.0        10.0         16.0          240         120
000                25           5             5          10
000                 8           4
000         1.8          1.8          1.5          1.5          1.5
000
000    @END
000    @PCH,S    TEMP.PCH
```

```
(.DECK
5-01/28-11:47
```

APPENDIX B

TWO-ELECTRODE PROGRAM

See Section 4, Figure 4.1 for diagram of structure. See end of Section 4 for description of data cards. End of listing gives example.

```
X,DECK,,MINE
B69      01/28-11:49:52

000    @RUN     CCD2,EE0017U,JIM,,/50
000    @ASG,T   TEMP,F2
000    @ELT,LIB TEMP.PCH
000    C*************************************************************
000    C     PROGRAM NUMBER 2******PERIODIC BOUNDARY CONDITIONS*********
000    C************** TWO OXIDE THICKNESSES ARE ALLOWABLE***************
000    C     *************************************************
000    C     ELECTROSTATIC ANALYSIS OF CCD STRUCTURE
000    C     DIMENSION ARRAYS, DEFINE COMMON VARIABLES
000    C      H IS THE GRID SPACING NORMAL TO THE INTERFACE
000    C      W   '   '   '   PARALLEL WITH THE INTERFACE
000    C      U IS THE ELECTROSTATIC POTENTIAL WRT THE SUBSTRATE BULK
000    C      DU IS THE RESIDUAL
000    C     *************************************************
000           COMMON U(100,110),DU(100),H(100),FO,L2,ALPHA,
000          *EA,EB,A,B,C,G,W,VT,SIGN,DROW,DUMAX,ABMAX,
000          *I,J,IMAX,JMAX,IM,I5
000           DIMENSION QS(100),CHION(11),ARRAY(100)
000           SIGMA=0.1
000           YBAR=-0.2
000           VT=0.0259
000           READ(5,1) JA,JB,JC,MAXU,IRES
000       1   FORMAT(5I10)
000    C     *************************************************
000    C      READ DIMENSIONS OF REGION FOR ANALYSIS, MICRONS
000    C     *************************************************
000    C     TOX1= THIN OXIDE THICKNESS.
000    C     TOX2= THICK OXIDE THICKNESS
000    C      TEL= ELECTRODE THICKNESS
000           READ(5,2) TOX1,TOX2,TEL,W,HFAC,HDEBY
000       2   FORMAT(6F10.3)
000    C     *************************************************
000    C     READ CHARGE DENSITY DATA
000    C     QG= GAP DOPING,POSITIVE IF SAME POLARITY AS QSS.
000    C     QP= UNDERPAD IMPLANTED DOPING,POSITIVE IF SAME POLARITY AS QSS.
000    C      QSS= SURFACE STATE CHARGE,CM-2
000    C     QU= UNIFORM IMPLANTED LAYER DENSITY,CM-2
000    C      CSUB= SUBSTRATE DOPING,CM-3
000           READ(5,4) QSS,CSUB,QG,QP,QU
000       4   FORMAT(5E10.3)
000    C*************************************************************
000    C   'SIGN' IS USED TO PRECLUDE SPACE CHARGE INSTABILITY IN RELAXATION
000    C    IN SUBSTRATE. IF 'U' HAS WRONG SIGN, 'U' IS SET TO ZERO.
000           SIGN=-1.0
000           IF(CSUB.GT.0.0)  SIGN = 1.0
000    C     *************************************************
000    C     *************************************************
000    C      COMPUTE CHARGE DENSITY PARAMETERS
000    C     *************************************************
000           Q=1.6E-19
000           EO=8.85E-14
000           VSS=Q*QSS/EO*1.E-4
000           VSUB=-Q*CSUB/EO*1.E-8
000           CON=2.*11.7E+8*EO/(Q*CSUB)
```

```
000          CO1=3.9E+4*EO/TOX1
000          CO2=3.9E+4*EO/TOX2
000     C    ***************************************************************
000     C    READ ELECTRODE VOLTAGES,NUMBER OF ITERATIONS,AND LOOP PRINTOUT
000     C    ***************************************************************
000          READ(5,6) V1,V2,ITER,LAP
000        6 FORMAT(2F10.3,2I10)
000     C    ***************************************************************
000     C     DETERMINE LATERAL CONTROL INDICES
000     C    THEN COMPUTE THE SURFACE CHARGE DISTRIBUTION
000     C    ***************************************************************
000     C    LP AND LG ARE THE NUMBER OF STEPS ACROSS THE PAD AND GAP.
000     C*****************IMPORTANTEEE IMPORTANTEEE ******************
000     C**********   LG MUST BE AN EVEN NUMBER    ******************
000     C    LDOPE= NUMBER OF STEPS ACROSS THE IMPLANTED REGION
000     C    LSPAC = NUMBER OF STEPS DOPING STARTS FROM THE LEFT EDGE OF
000     C              THE ELECTRODE,  POSITIVE IS TO THE RIGHT.
000     C    LOX1= NUMBER OF STEPS ACROSS THE THIN OXIDE.
000     C    LSPOX= NUMBER OF STEPS THE THIN OXIDE STARTS FROM THE LEFT EDGE
000     C              OF THE ELECTRODE,  POSITIVE TO THE RIGHT.
000     C*************************************************************
000          READ(5,18)LP,LG,LDOPE,LSPAC,LOX1,LSPOX
000       18 FORMAT(6I10)
000          I1=LG/2+1
000          I2=I1+LP
000          I3=I2+LG
000          I4=I3+LP
000          I5=I4+LG/2
000          IA=I1+LSPAC
000          IB=IA+LDOPE
000          IC=(I2+I3)/2
000          ID=I3+LSPAC
000          IE=ID+LDOPE
000          IF=I1+LSPOX
000          IG=IF+LOX1
000          IH=I3+LSPOX
000          IK=IH+LOX1
000          IL1=IF
000          IF(I1.GT.IF) IL1=I1
000          IR1=I2
000          IF(I2.GT.IG) IR1=IG
000          IL2=IH
000          IF(I3.GT.IH) IL2=I3
000          IR2=I4
000          IF(I4.GT.IK) IR2=IK
000          DO 333 I=2,I5
000          QS(I)=QG*(F(1,I1,I)+F(I2,I3,I)+F(I4,I5,I))
000         *+QP*(F(IA,IB,I)+F(ID,IE,I))+QU
000       333 CONTINUE
000          QS(1)=QG
000          QS(IA)=QS(IA)-QP/2.
000          QS(IB)=QS(IB)-QP/2.
000          QS(ID)=QS(ID)-QP/2.
000          QS(IE)=QS(IE)-QP/2.
000          QS(I1)=QS(I1)-QG/2.
000          QS(I2)=QS(I2)-QG/2.
000          QS(I3)=QS(I3)-QG/2.
```

```
000          QS(I4)=QS(I4)-QG/29
000     C    ***************************************************************
000     C     FIND THE EXTRINSIC DEBYE LENGTH
000     C    ***************************************************************
000          DL=VT*11.7*EO/Q/CSUB
000          EDL=SQRT(DL)*1.E4
000     C    ***************************************************************
000     C     DETERMINE NORMAL CONTROL INDICES
000     C     AND SET THE Y-GRID SPACING
000     C    L1=NUMBER OF UNIFORM STEPS THROUGH SEMICONDUCTOR.
000     C    L2=   '    '   EXPONENTIAL    '          '    '
000     C    L3=  '      '    UNIFORM STEPS THROUGH THIN OXIDE
000     C    L4=  '    '          '          '   ELECTRODE REGION.
000     C    L5=   '    '    EXPONENTIAL STEPS IN THE AIRSPACE REGION.
000     C    ***************************************************************
000          READ(5,302)  L1,L3,L4,L5
000      302 FORMAT(4I10)
000          J1=L1+1
000          K1=L1
000          HO=3.*TOX1/L3
000          IF(HO.GT.EDL) HO=EDL
000          IF(HDEBY.LT.2.) HDEBY=2.0
000          YO=HDEBY*EDL
000          FO=YO/HO
000          CALL YSPAC
000          J2=J1+L2
000          K2=J2-1
000          DO 10 JJ=1,L2
000          J=J2-JJ
000          H(J)= HO*ALPHA**JJ
000       10 CONTINUE
000          J3=J2+L3
000          K3=J3-1
000          DO 12 J=J2,K3
000          HOX=TOX1/L3
000          H(J)=HOX
000       12 CONTINUE
000          ITOX=(TOX2-TOX1)/HOX
000          IF(ITOX.GT.0)  HT=(TOX2-TOX1)/ITOX
000          J4=J3+ITOX
000          K4=J4-1
000          IF(ITOX.EQ.0) GO TO 14
000          DO 21 J=J3,K4
000          H(J)=HT
000       21 CONTINUE
000          J5=J4+L4
000          K5=J5-1
000       14 DO 15 J=J4,K5
000          H(J)=TEL/L4
000       15 CONTINUE
000          J6=J5+L5
000          K6=J6-1
000          DO 16 J=J5,K6
000          JJ=J-J5
000          H(J)=(TEL/L4)*(2.**JJ)
000       16 CONTINUE
000     C    ***************************************************************
```

```
000    C       SET THE ELECTRODE POTENTIALS
000    C       ****************************************************************
000            DO 28 J=J3,J5
000            DO 26 I=I1,I4
000            IF(ITOX.EQ.0) GO TO 24
000            IF(J.GE.J4) GO TO 24
000            U(I,J)=V1*F(IL1,IR1,I)+V2*F(IL2,IR2,I)
000            GO TO 26
000       24   U(I,J)=V1*F(I1,I2,I)+V2*F(I3,I4,I)
000       26   CONTINUE
000       28   CONTINUE
000    C       ****************************************************************
000    C       ESTIMATE DEPLETION DEPTH
000    C       ESTIMATE SURFACE POTENTIAL
000    C       ****************************************************************
000            DO 399 I=1,I5
000            IF(I.LT.I1.AND.I.GE.1) GO TO 398
000            IF(I.LT.I3.AND.I.GT.I2) GO TO 398
000            IF(I.LE.I5.AND.I.GT.I4) GO TO 398
000            CO=CO2
000            IF(I.GE.IF.AND.I.LE.IG) CO=CO1
000            IF(I.GE.IH.AND.I.LE.IK) CO=CO1
000            VA=U(I,J4)+Q*(QSS+QS(I))/CO
000            VB=Q*CSUB/CO*11.7*EO/CO
000            U(I,J2)=VA+VB-SQRT(2.*VA*VB+VB**2)
000            GO TO 399
000       398  U(I,J2)=Q*((QS(I)+QSS)**2)/(2.*11.7*EO*CSUB)
000       399  CONTINUE
000            VINT=0.0
000            DO 397 I=2,I5
000            PSI=ABS((U(I,J2)+U(I-1,J2))/2.0)
000            IF(PSI.GT.VINT) VINT=PSI
000       397  CONTINUE
000            XDS=ABS(CON*VINT)
000            XD=SQRT(XDS)
000    C       ****************************************************************
000    C       SET DEFAULT VALUE FOR HFAC
000    C       ****************************************************************
000            IF(HFAC.LT.1.0) HFAC=2.0
000            DO 8 J=1,K1
000            H(J)=HFAC*XD/L1
000       8    CONTINUE
000    C       ****************************************************************
000    C       WRITE DEPLETION DEPTH AND DEBYE LENGTH
000    C       ****************************************************************
000            WRITE(6,300) XD,EDL
000       300  FORMAT('1',10X,'DEPLETION DEPTH =',F10.3,5X,'DEBYE LENGTH=',F10.3)
000    C       ****************************************************************
000    C       PRINT OUT THE Y-COORDINATE VALUES AND THECONTROL INDICES
000    C       ****************************************************************
000            WRITE(6,601)
000       601  FORMAT(10X,'THE Y-COORDINATE VALUES ARE AS FOLLOWS:',//)
000            Y=0.
000            DO 125 J=J2,K6
000            Y=Y+H(J)
000            WRITE(6,126) Y
000       125  CONTINUE
```

```
000           Y=0.
000           DO 127  LL=1,K2
000           J=J2-LL
000           Y=Y-H(J)
000           WRITE(6,126) Y
000     126   FORMAT(F20.6)
000           IF(LL.GT.10) GO TO 127
000           EXPO=(Y-YBAR)**2/(4.*SIGMA**2)
000           CHION(LL)=EXP(-EXPO)*(H(J)+H(J-1))/2.0
000     127   CONTINUE
000     C     ***************************************************************
000     C       THE FOLLOWING GIVES THE WEIGHT OF THE IMPLANTED SURFACE CHARGE
000     C       WHICH IS TO BE USED AT POINTS BELOW THE INTERFACE.
000     C     ***************************************************************
000           SUM=0.0
000           DO 128 LL=1,10
000           SUM=SUM+CHION(LL)
000     128   CONTINUE
000           DO 129 LL=1,10
000           CHION(LL)=CHION(LL)/SUM
000     129   CONTINUE
000           WRITE(6,131) J1,J2,J3,J4,J5,J6
000     131   FORMAT(//,10X,'J-VALUES ARE:',6I10//)
000     C     ***************************************************************
000     C       COMPUTE JA,JB VALUES WHICH WILL GIVE PRINTOUT OF THE INTERFACE
000     C     POTENTIAL DISTRIBUTION.
000     C     ***************************************************************
000           MT=(J2-JA)/JC
000           JA=J2-MT*JC
000           IF(JB.GT.J5) JB=J5
000     C     ***************************************************************
000     C     INITIALIZE POTENTIAL DISTRIBUTION IN THE SEMICONDUCTOR AND
000     C      OXIDE USING THE ONE DIMENSIONAL DEPLETION LAYER ESTIMATE.
000     C     ***************************************************************
000           DO 406 I=2,I5
000           IRITE=I+1
000           IF(I.EQ.I5) IRITE=I2
000           VINT=U(I-1,J2)/4.+U(I,J2)/2.+U(IRITE,J2)/2.
000           XDS=ABS(CON*VINT)
000           XD=SQRT(XDS)
000           Y=0.0
000           J=J2
000     400   J=J-1
000           IF(J.LE.1) GO TO 402
000           Y=Y+H(J)
000           YN=Y/XD
000           IF(YN.GE.1.0) GO TO 402
000           U(I,J)=U(I,J2)*(1.0-YN)**2
000           GO TO 400
000     402   JJ=J2+1
000           IF(I.GE.IL1.AND.I.LE.IR1) GO TO 404
000           IF(I.GE.IL2.AND.I.LE.IR2) GO TO 404
000           DO 403 J=JJ,K4
000           U(I,J)=U(I,J2)
000     403   CONTINUE
000           GO TO 406
000     404   DO 405 J=JJ,K3
```

```
000          U(I,J)=U(I,J2)
000      405 CONTINUE
000      406 CONTINUE
000     C*****************************************************************
000     C     WRITE OUT THE STRUCTURE PARAMETERS.
000     C*****************************************************************
000          WRITE(6,345) TOX1,TOX2,TEL,W,V1,V2,LP,LG,LDOPE,LSPAC,LOX1,LSPOX,
000         *QSS,QG,QP,CSUB
000      345 FORMAT(/,10X,'(TOX1,TOX2,TEL,W)=',4F10.3,/,10X,'(V1,V2)=',2F10.3,
000         */,10X,'(LP,LG,LDOPE,LSPAC,LOX1,LSPOX)=',6I6,/
000         *,10X,'(QSS,QG,QP,CSUB)=',4E10.3//)
000          WRITE(6,206) (U(I,J2),I=1,IC)
000          WRITE(6,206) (U(I,J2),I=IC,I5)
000     C    *****************************************************************
000     C    READ RELAXATION PARAMETER VALUES
000     C    *****************************************************************
000          READ(5,408) OM1,OM2,OM3,OM4,OM5
000      408 FORMAT(5F10.3)
000          KT=1
000          JLO=2
000          JHI=J5+1
000     C    *****************************************************************
000     C     START THE RELAXATION PROCEDURE STARTING AT THE LOWEST ROW
000     C     AND WORKING ACROSS TO THE RIGHT TO THE TOP ROW
000     C    *****************************************************************
000          LOOP=1
000      800 CONTINUE
000          DUMAX=0.0
000          ABMAX=0.0
000          DO 40 J=JLO,K2
000          EA=11.7
000          EB=11.7
000          CALL COEFF
000          OMEGA=OM1
000          DO 38 I=2,I5
000          ITEST=1
000          IF(U(I,J+1).EQ.0.0) GO TO 33
000       30 LL=J2-J
000          IF(LL.GT.10) GO TO 32
000          QIMP=QS(I)*CHION(LL)
000          QIJ=VSUB*AVERO(ITEST)+1.E-4*Q*QIMP*W/EO
000          GO TO 35
000       32 QIJ=VSUB*AVERO(ITEST)
000       35 CALL RELAX(QIJ,OMEGA)
000          US=SIGN*U(I,J)
000          IF(US.LT.0.0) U(I,J)=0.0
000          GO TO 38
000       33 IF(U(I+1,J).EQ.0.0) GO TO 34
000          GO TO 30
000       34 IF(U(I-1,J).EQ.0.0) GO TO 38
000       38 CONTINUE
000          CALL MAXOF
000          U(1,J)=U(I5,J)
000          MAX=1000*ABMAX
000          IF(J.EQ.JLO.AND.MAX.GT.0) JLO=J-1
000          IF(MAX.EQ.0) JLO=J
000          IF(JLO.LT.2) JLO=2
```

```
000      40  CONTINUE
000     C    ************************************************************
000     C     RELAX THE SILICON,SILICON-DIOXIDE INTERFACE
000     C    ************************************************************
000          J=J2
000          EA=11.7
000          EB=3.9
000          CALL COEFF
000          OMEGA=OM2
000          DO 48 I=2,I5
000      42  QIJ=VSUB*H(J-1)*W/2.+1.E-4*Q*QSS*W/EO
000          CALL RELAX(QIJ,OMEGA)
000      48  CONTINUE
000          CALL MAXOF
000          U(1,J)=U(I5,J)
000     C************************************************************
000     C    NEXT STEP GIVES PRINTOUT OF THE INTERFACE RESIDUALS
000     C    ************************************************************
000          IF(IRES.GT.0) WRITE(6,697) DROW,IM
000     C    ************************************************************
000     C     RELAX THE OXIDE REGION
000     C    ************************************************************
000          JJ=J2+1
000          DO 60 J=JJ,K4
000          EA=3.9
000          EB=3.9
000          CALL COEFF
000          KSET=1
000          IF(ITOX.EQ.0) GO TO 49
000          IF(J.GE.J3) KSET=0
000      49  OMEGA=OM3
000          U(1,J)=U(I5,J)
000          QIJ=0.0
000          DO 58 I=2,I5
000          IF(KSET.EQ.1) GO TO 52
000          IF(I.GE.IL1.AND.I.LE.IR1) GO TO 58
000          IF(I.GE.IR1.AND.I.LE.IR2) GO TO 58
000      52  CALL RELAX(QIJ,OMEGA)
000      58  CONTINUE
000          CALL MAXOF
000      60  CONTINUE
000     C    ************************************************************
000     C    RELAX THE OXIDE-AIR INTERFACE
000     C    ************************************************************
000          J=J4
000          EA=3.9
000          EB=1.0
000          CALL COEFF
000          QIJ=0.
000          DO 68 I=2,I5
000          IF(I.GE.I1.AND.I.LE.I2) GO TO 68
000          IF(I.GE.I3.AND.I.LE.I4) GO TO 68
000          OMEGA=OM4
000          CALL RELAX(QIJ,OMEGA)
000      68  CONTINUE
000          CALL MAXOF
000          U(1,J)=U(I5,J)
```

```
000   C     ************************************************************
000   C      RELAX THE ELECTRODE-AIRSPACE REGION
000   C     ************************************************************
000         JJ=J4+1
000         DO 80 J=JJ,K5
000         EA=1.
000         EB=1.
000         CALL COEFF
000         OMEGA=OM5
000         QIJ=0.
000         DO 78 I=2,I5
000         IF(I.GE.I1.AND.I.LE.I2) GO TO 78
000         IF(I.GE.I3.AND.I.LE.I4) GO TO 78
000         CALL RELAX(QIJ,OMEGA)
000      78 CONTINUE
000         CALL MAXOF
000         U(1,J)=U(I5,J)
000      80 CONTINUE
000   C     ************************************************************
000   C      RELAX THE AIR-SPACE REGION ABOVE THE ELECTRODES
000   C     ************************************************************
000         JJ=J5+1
000         DO 90 J=JJ,JHI
000         EA=1.
000         EB=1.
000         CALL COEFF
000         OMEGA=OM5
000         QIJ=0.
000         DO 88 I=2,I5
000         CALL RELAX(QIJ,OMEGA)
000      88 CONTINUE
000         CALL MAXOF
000      90 CONTINUE
000         JHI=JHI+1
000         IF(JHI.GT.K6) JHI=K6
000         IF(IRES.GT.0) WRITE(6,212) DUMAX,IMAX,JMAX,JLO
000   C     ************************************************************
000   C     OUTPUT CONTROL AND ITERATION CONTROL FOLLOWS
000   C     THIS ITERATION CONTROL CAN BE REPLACED BY A CONDITIONAL
000   C     CONTROL ON EITHER DU OR DUMAX.
000   C     ************************************************************
000         LWRIT=LOOP/LAP
000         IF(LWRIT.EQ.KT) GO TO 881
000     207 CONTINUE
000         LOOP=LOOP+1
000         IF(LOOP.LE.ITER) GO TO 800
000   C  ************************************************************
000   C     THE FOLLOWING READ MAY BE USED FOR FINDING NEW POTENTIALS
000   C     AFTER APPLYING PERTURBATIONS TO THE ELECTRODE VOLTAGES.
000   C  ************************************************************
000         READ(5,6) V1,V2,ITER,LAP
000         IF(ITER.EQ.0) STOP
000         DO 883 J=J3,J5
000         DO 882 I=I1,I4
000         IF(J.GE.J4) GO TO 880
000         U(I,J)=V1*F(IL1,IR1,I)+V2*F(IL2,IR2,I)+(1.-F(IL1,IR1,I)
000        *-F(IL2,IR2,I))*U(I,J)
```

```
000          GO TO 882
000     880  U(I,J)=V1*F(I1,I2,I)+V2*F(I3,I4,I)+(1.-F(I1,I2,I)
000         *-F(I3,I4,I))*U(I,J)
000     882  CONTINUE
000     883  CONTINUE
000          LOOP=1
000          KT=1
000          GO TO 800
000     C*****************************************************************
000     C    DO 205 J=JA,JB,JC CONTROLS THE OUTPUT WRITE.  PRINTOUT STARTS
000     C    ON LINE JA AND GOES TO LINE JB IN STEPS OF SIZE JC.
000      881 CONTINUE
000          WRITE(6,697) DROW,IM
000     697  FORMAT(2X,'RI=',F5.3,5X,'I=',I3)
000          WRITE(6,212) DUMAX,IMAX,JMAX,JLO
000     212  FORMAT(30X,' RMAX=',F10.3,5X,'IMAX=',I4,5X,'JMAX=',I4,5X,'JLO='
000         *,I4)
000          DO 205 J=JA,JB,JC
000          WRITE(6,208) J
000     208  FORMAT(10X,'J=',I3)
000          WRITE(6,206) (U(I,J), I=1,IC)
000          WRITE(6,206) (U(I,J), I=IC,I5)
000     206  FORMAT(10F10.2)
000     205  CONTINUE
000          IF(MAXU.EQ.0) GO TO 516
000          DO 506 I=1,I5
000          AUMAX=0.0
000          LMAX=0
000          DO 504 J=1,J2
000          ABU=ABS(U(I,J))
000          IF(ABU.GT.AUMAX) GO TO 502
000          GO TO 504
000     502  AUMAX=ABU
000          LMAX=J2-J
000     504  CONTINUE
000          DU(I)=LMAX
000          JM=J2-LMAX
000          ARRAY(I)=U(I,JM)
000     506  CONTINUE
000          WRITE(6,508)
000     508  FORMAT(/,10X,'THE NUMBER OF STEPS UMAX OCCURS BELOW SURFACE IS:'/)
000          WRITE(6,206) (DU(I),I=1,IC)
000          WRITE(6,206) (DU(I),I=IC,I5)
000          WRITE(6,510)
000     510  FORMAT(/,10X,'THE MAX POTENTIALS ARE:'/)
000          WRITE(6,206) (ARRAY(I),I=1,IC)
000          WRITE(6,206) (ARRAY(I),I=IC,I5)
000     516  KT=KT+1
000          GO TO 207
000          END
000          FUNCTION F(II,JJ,KK)
000          F=0.0
000          IF(KK.GE.II.AND.KK.LE.JJ) F=1.0
000          RETURN
000          END
000          SUBROUTINE YSPAC
000          COMMON U(100,110),DU(100),H(100),FO,L2,ALPHA,
```

```
000          *EA,EB,A,B,C,G,W,VT,SIGN,DROW,DUMAX,ABMAX,
000          *I,J,IMAX,JMAX,IM,I5
000           ALPHA=1.25
000           L2=ALOG(0.25*F0+1.0)/ALOG(ALPHA)
000       2   F1=(ALPHA**L2-1.)/(ALPHA-1.)
000           TRY=ABS(F1/F0)
000           IF(TRY.LT.1.005.AND.TRY.GT.0.995) GO TO 4
000           F=F1-F0
000           LL=L2-1
000           F3=L2*(ALPHA**LL)/(ALPHA-1.)
000           F4=(ALPHA**L2-1.)/((ALPHA-1.)**2)
000           FP=F3-F4
000           ALPHA=ALPHA-F/FP
000           GO TO 2
000       4   CONTINUE
000           RETURN
000           END
000           SUBROUTINE COEFF
000           COMMON U(100,110),DU(100),H(100),F0,L2,ALPHA,
000          *EA,EB,A,B,C,G,W,VT,SIGN,DROW,DUMAX,ABMAX,
000          *I,J,IMAX,JMAX,IM,I5
000           A=EA*W/H(J-1)
000           B=(EA*H(J-1)+EB*H(J))/(2.*W)
000           G=EB*W/H(J)
000           C=A+2.*B+G
000           RETURN
000           END
000           FUNCTION AVERO(ITEST)
000           COMMON U(100,110),DU(100),H(100),F0,L2,ALPHA,
000          *EA,EB,A,B,C,G,W,VT,SIGN,DROW,DUMAX,ABMAX,
000          *I,J,IMAX,JMAX,IM,I5
000           S=0.0
000           U1=ABS(U(I,J)+U(I,J-1))
000           IF(U1.GT.0.0) S=0.5*H(J-1)
000           IF(ITEST.GT.2) GO TO 4
000           U2=ABS(U(I,J)+U(I,J+1))
000           IF(U2.GT.0.0) S=S+0.5*H(J)
000       4   AVERO=S*W
000           RETURN
000           END
000           SUBROUTINE RELAX(QIJ,OMEGA)
000           COMMON U(100,110),DU(100),H(100),F0,L2,ALPHA,
000          *EA,EB,A,B,C,G,W,VT,SIGN,DROW,DUMAX,ABMAX,
000          *I,J,IMAX,JMAX,IM,I5
000           UOLD=U(I,J)
000           IRITE=I+1
000           IF(I.EQ.I5) IRITE=2
000           UTIL=(A*U(I,J-1)+B*U(I-1,J)+B*U(IRITE,J)+G*U(I,J+1)+QIJ)/C
000           U(I,J)=(1.-OMEGA)*UOLD+OMEGA*UTIL
000       2   DU(I)=U(I,J)-UOLD
000           RETURN
000           END
000           SUBROUTINE MAXOF
000           COMMON U(100,110),DU(100),H(100),F0,L2,ALPHA,
000          *EA,EB,A,B,C,G,W,VT,SIGN,DROW,DUMAX,ABMAX,
000          *I,J,IMAX,JMAX,IM,I5
000           DAB=0.0
```

```
000           DROW=0.0
000           DO 4 I=2,I5
000           ABDU=ABS(DU(I))
000           IF(ABDU.GT.DAB) GO TO 2
000           GO TO 4
000       2   DAB=ABDU
000           DROW=DU(I)
000           IM=I
000       4   CONTINUE
000           IF(DAB.GT.ABMAX) GO TO 6
000           GO TO 8
000       6   ABMAX=DAB
000           DUMAX=DROW
000           IMAX=IM
000           JMAX=J
000       8   RETURN
000           END
000   @XQT
000              15          80          5          1
000       0.100     0.500       0.800      1.00
000       2.00E+11  3.80E+15                1.38E+12  4.70E+11
000         1.0       20.           240        120
000              16          8          8          9          8          9
000              25          4         10         10
000         1.8       1.8        1.5        1.5        1.5
000
000   @END
000   @PCH,S   TEMP.PCH
```

```
 X.DECK
26-01/28-11:50
```

APPENDIX C

FOUR-ELECTRODE PROGRAM

See Section 5, Figure 5.1 for diagram of structure. See end of Section 5 for description of data cards. End of listing gives example.

```
X,DECK,,MINE
B69      01/28-11:49:03

000    @RUN    CCD2,EE0017U,JIM,,/50
000    @ASG,T   TEMP,F2
000    @ELT,LIB TEMP.PCH
000    C      ********************************************************
000    C                   PROGRAM NO. 3
000    C       ELECTROSTATIC ANALYSIS OF A CHARGE COUPLED STRUCTURE
000    C      ********************************************************
000    CC                    FOUR ELECTRODE CELL
000    C               ITYPE=0   :  SAPPHIRE SUBSTRATE
000    C               ITYPE GT. 0 :   SILICON SUBSTRATE
000    C      ********************************************************
000    C       DIMENSION ARRAYS
000    C      ********************************************************
000           COMMON U(100,100),DU(100),H(100),A,B,C,G,W,EA,EB,DROW,DUMAX,QSUB
000          *,ABMAX,I,J,IMAX,JMAX,IM,I5
000           DIMENSION DUM(100),QIMP(100)
000    C      ********************************************************
000    C      LG1 AND LP2 MUST BE EVEN NUMBERS.
000    C      LG1 AND LP1 : GAP AND ELECTRODE WIDTH IN UNITS OF W,BOTTOM.
000    C      LG2 AND LP2:    '    '    '    '    '    '    ,TOP.
000    C      ********************************************************
000           READ(5,2) LP1,LG1,LP2,LG2,ITYPE,MAXU
000        2  FORMAT(6I10)
000    C      ********************************************************
000    C      L1 THROUGH L8 : NUMBER OF STEPS VERTICALLY THROUGH EACH OF
000    C      THE REGIONS DEFINEDON DIAGRAM OF STRUCTURE.
000    C      ********************************************************
000           READ(5,3) JA,JB,JC
000        3  FORMAT(3I10)
000           READ(5,4) L1,L2,L3,L4,L5,L6,L7,L8
000        4  FORMAT(4I10)
000    C      ********************************************************
000    C      TOX1,TEL1,TOX2,TEL2,TOX3,TSI,W: THICKNESSES OF THE OXIDE,
000    C      ELECTRODE,AND SILICON REGIONS IN MICRONS.
000    C      ********************************************************
000           READ(5,6) TOX1,TEL1,TOX2,TEL2,TOX3,TSI,W
000        6  FORMAT(4F10.3)
000    C      ********************************************************
000    C      QSS1,QSS2: SURFACE STATE CHARGE AT LOWER AND UPPER INTERFACES,CM-2
000    C      QUN: UNIFORM IMPLANTED ION DENSITY,CM-2.
000    C       CSUB: SUBSTRATE DOPING, POSITIVE FOR P-TYPE,CM-3.
000    C      ********************************************************
000           READ(5,8) QSS1,QSS2,QUN,CSUB
000        8  FORMAT(4E10.3)
000    C      ********************************************************
000    C      VG1,VG2,VG3,VG4 :  ELECTRODE VOLTAGES VOLTS.
000    C      ITER: TOTAL NO. OF ITERATIONS FOR SOLUTION.
000    C      LAP:  PRINTOUT ON ITER. NO. LOOP/LAP = INTEGER.
000    C      ********************************************************
000           READ(5,10) VG1,VG2,VG3,VG4,ITER,LAP
000       10  FORMAT(4F10.3,2I10)
000    C      ********************************************************
000    C      OMN IS THE RELAXATION PARAMETER IN REGION N.
000    C      YBAR AND SIGMA ARE THE PARAMETERS FOR THE IIMPLANTED DISTRIB.
```

```
000   C     **********************************************************************
000         READ(5,11) OM1,OM2,OM3,OM4,YBAR,SIGMA
000      11 FORMAT(6F10.3)
000         EO=8.854E-14
000         Q=1.6E-19
000         SIGN=1.0
000         IF(CSUB.LT.0.) SIGN=-1.0
000         I1=LG1/2+1
000         I2=I1+LP1
000         I3=I2+LG1
000         I4=I3+LP1
000         I5=I4+LG1/2
000         I6=LP2/2+1
000         I7=I6+LG2
000         I8=I7+LP2
000         I9=I8+LG2
000         IC=(I2+I3)/2
000         J1=L1+1
000         K1=J1-1
000         JJ1=J1+1
000         J2=J1+L2
000         K2=J2-1
000         JJ2=J2+1
000         J3=J2+L3
000         K3=J3-1
000         JJ3=J3+1
000         J4=J3+L4
000         K4=J4-1
000         JJ4=J4+1
000         J5=J4+L5
000         K5=J5-1
000         JJ5=J5+1
000         J6=J5+L6
000         K6=J6-1
000         JJ6=J6+1
000         J7=J6+L7
000         K7=J7-1
000         JJ7=J7+1
000         J8=J7+L8
000         K8=J8-1
000         YSUB=I5*W
000         IF(ITYPE.EQ.0) GO TO 13
000         ABVM=10.
000         ABV1=ABS(VG1)
000         ABV2=ABS(VG2)
000         ABV3=ABS(VG3)
000         ABV4=ABS(VG4)
000         IF(ABV1.GT.ABVM) ABVM=ABV1
000         IF(ABV2.GT.ABVM) ABVM=ABV2
000         IF(ABV3.GT.ABVM) ABVM=ABV3
000         IF(ABV4.GT.ABVM) ABVM=ABV4
000         VMAX=SIGN*ABVM
000         CSI=11.7E+4*EO/TSI
000         CO=3.9E+4*EO/(TOX1+TEL1+TOX2)
000         CTOT=CO*CSI/(CO+CSI)
000         QTOT=(QUN+QSS1-1.E-4*CSUB*TSI)*Q
000         VA=VMAX+QTOT/CTOT
```

```
000           VB=Q*CSUB*11.7*E0/(CTOT**2)
000           PSI=VA+VB-SQRT(2.*VA*VB+VB**2)
000           XDS=2.*11.7*E0*PSI/(Q*CSUB)
000           XD=1.E+4*SQRT(ABS(XDS))
000           YSUB=2.*XD
000      13   CONTINUE
000           DO 12 J=J2,K3
000           H(J)=TOX1/L3
000      12   CONTINUE
000           DO 14  J=J3,K4
000           H(J)=TEL1/L4
000      14   CONTINUE
000           DO 16 J=J4,K5
000           H(J)=TOX2/L5
000      16   CONTINUE
000           DO 18 J=J5,K6
000           H(J)=TEL2/L6
000      18   CONTINUE
000           DO 20 J=J6,K7
000           H(J)=TOX3/L7
000       20  CONTINUE
000           DO 22 J=J7,K8
000           H(J)=0.25*H(K7)*1.5**(J-J7)
000      22   CONTINUE
000           DO 24 J=J1,K2
000           H(J)=TSI/L2
000       24  CONTINUE
000           HSAP=TSI/L2*12.3/11.7
000           ALPHA=1.25
000           F0=YSUB/HSAP
000      26   F1=(ALPHA**L1-1.)/(ALPHA-1.)
000           TRY=ABS(F1/F0)
000           IF(TRY.LT.1.005.AND.TRY.GT..995) GO TO 28
000           FA=F1-F0
000           LL=L1-1
000           F3=L1*ALPHA**LL/(ALPHA-1.)
000           F4=(ALPHA**L1-1.)/((ALPHA-1.)**2)
000           FP=F3-F4
000           ALPHA=ALPHA-FA/FP
000           GO TO 26
000      28   CONTINUE
000           DO 30 LL=1,K1
000           J=J1-LL
000           H(J)=HSAP*ALPHA**LL
000      30   CONTINUE
000           WRITE(6,32)
000      32   FORMAT(/,10X,'THE Y-VALUES ARE:',/)
000           Y=0.0
000           DO 36 J=J2,K8
000           WRITE(6,34) Y
000      34   FORMAT(10X,F10.3)
000           Y=Y+H(J)
000           DUM(J)=Y
000      36   CONTINUE
000           Y=0.0
000           DO 38 LL=1,L2
000           J=J2-LL
```

```
000           WRITE(6,34) Y
000           Y=Y-H(J)
000           DUM(J)=Y
000           QIMP(LL)=DISF(Y,YBAR,SIGMA)*(H(J)+H(J-1))/2.
000        38 CONTINUE
000           DO 40 LL=1,L1
000           WRITE(6,34) Y
000           J=J1-LL
000           Y=Y-H(J)
000           DUM(J)=Y
000        40 CONTINUE
000           SUM=0.0
000           DO 42 LL=1,L2
000           SUM=SUM+QIMP(LL)
000        42 CONTINUE
000           DO 44 LL=1,L2
000           QIMP(LL)=QUN*QIMP(LL)/SUM
000        44 CONTINUE
000           DO 48 J=J1,J7
000           DO 46 I=1,I5
000           U(I,J)=VG3*(F(1,I6,I)+F(I9,I5,I))+VG4*F(I7,I8,I)
000        46 CONTINUE
000        48 CONTINUE
000           DO 52 J=J1,K5
000           DO 50 I=1,I5
000           U(I,J)=VG1*F(I1,I2,I)+VG2*F(I3,I4,I)
000        50 CONTINUE
000        52 CONTINUE
000           IF(ITYPE.GT.0) GO TO 57
000           BETA=6.28/(I5*W)
000           DO 56 J=2,K1
000           Y=DUM(J)
000           EXPO=EXP(BETA*Y)
000           DO 54 I=1,I5
000           U(I,J)=U(I,J1)*EXPO
000        54 CONTINUE
000        56 CONTINUE
000        57 CONTINUE
000           WRITE(6,500)  J1,J2,J3,J4,J5,J6,J7,J8
000       500 FORMAT(/,10X,'(J1,J2,J3,J4,J5,J6,J7,J8)=',8I5)
000           WRITE(6,502) LP1,LG1,LP2,LG2
000       502 FORMAT(/,10X,'(LP1,LG1,LP2,LG2)=',4I5/)
000           WRITE(6,504) TOX1,TEL1,TOX2,TEL2,TOX3,TSI,W
000       504 FORMAT(/,10X,'(TOX1,TEL2,TOX2,TEL2,TOX3,TSI,W)=',7F6.3/)
000           WRITE(6,506) QSS1,QSS2,QUN,CSUB
000       506 FORMAT(/,10X,'(QSS1,QSS2,QUN,CSUB)=',4E10.3/)
000           WRITE(6,508) VG1,VG2,VG3,VG4
000       508 FORMAT(/,10X,' (VG1,VG2,VG3,VG4)=',4F10.3,/)
000           WRITE(6,510) ITER,LAP,YBAR,SIGMA
000       510 FORMAT(/,10X,'(ITER,LAP,YBAR,SIGMA)=',2I8,2F10.3,/)
000           WRITE(6,512) OM1,OM2,OM3,OM4
000       512 FORMAT(/,10X,'(OM1,OM2,OM3,OM4)=',4F10.3,/)
000           MSTEP=(J2-JA)/2
000           JA=J2-MSTEP*JC
000           IF(JA.LT.1) JA=1
000           IF(JB.GT.J8) JB=J8
000     C     ********************************************************
```

```
000   C     RELAX  THE SUBSTRATE REGION (SAPPHIRE OR SILICON)
000   C     ********************************************************************
000         JLO=K1-3
000         JHI=J7+1
000         LOOP=1
000         KT=1
000    1000 CONTINUE
000         JLO=JLO-1
000         JHI=JHI+1
000         IF(JLO.LT.2) JLO=2
000         IF(JHI.GT.K8) JHI=K8
000         DUMAX=0.
000         ABMAX=0.
000         IF(ITYPE.EQ.0) GO TO 660
000         DO 700 J=JLO,J1
000         EA=11.7
000         EB=11.7
000         OMEGA=OM1
000         CALL COEFF
000         DO 680 I=2,I5
000         CALL AVERO
000         QIJ=-1.E-8*Q*QSUB*CSUB/E0
000         CALL RELAX(QIJ,OMEGA)
000         UTEST=SIGN*U(I,J)
000         IF(UTEST.LT.0.) U(I,J)=0.
000     680 CONTINUE
000         CALL MAXOF
000         U(1,J)=U(I5,J)
000     700 CONTINUE
000         GO TO 720
000     660 DO 70 J=JLO,K1
000         EA=12.3
000         EB=12.3
000         OMEGA=OM1
000         CALL COEFF
000         QIJ=0.
000         DO 68 I=2,I5
000         CALL RELAX(QIJ,OMEGA)
000      68 CONTINUE
000         CALL MAXOF
000         U(1,J)=U(I5,J)
000      70 CONTINUE
000   C     ********************************************************************
000   C     RELAX SAPPHIRE-SILICON INTERFACE
000   C     ********************************************************************
000         J=J1
000         LL=J-J2
000         EA=12.3
000         EB=11.7
000         OMEGA=OM1
000         CALL COEFF
000         QIJ=1.E-4*Q*(QIMP(LL)/2.-1.E-4*CSUB*H(J)+QSS2)*W/E0
000         DO 72 I=2,I5
000         CALL RELAX(QIJ,OMEGA)
000      72 CONTINUE
000         CALL MAXOF
000         U(1,J1)=U(I5,J1)
```

```
000   C     ***********************************************************
000   C      RELAX THE IMPLANTED SILICON REGION.
000   C     ***********************************************************
000    720  DO 76 J=JJ1,K2
000         EA=11.7
000         EB=11.7
000         OMEGA=OM2
000         LL=J2-J
000         QIJ=1.E-4*Q*(QIMP(LL)-1.E-4*CSUB*(H(J)+H(J-1))/2.)*W/EO
000         DO 74 I=2,I5
000         CALL RELAX(QIJ,OMEGA)
000      74 CONTINUE
000         CALL MAXOF
000         U(1,J)=U(I5,J2)
000      76 CONTINUE
000   C     ***********************************************************
000   C     RELAX THE SILICON-SI-02 INTERFACE.
000   C     ***********************************************************
000         J=J2
000         EA=11.7
000         EB=3.9
000         OMEGA=OM2
000         CALL COEFF
000         LL=J-J2
000         QIJ=1.E-4*Q*(QIMP(LL)-1.E-4*CSUB*H(J-1)/2.+QSS1)*W/EO
000         DO 78 I=2,I5
000         CALL RELAX(QIJ,OMEGA)
000      78 CONTINUE
000         CALL MAXOF
000         U(1,J2)=U(I5,J2)
000         WRITE(6,320) DROW,IM
000    320  FORMAT(10X,'RI=',F8.3,5X,'IM=',I4)
000   C     ***********************************************************
000   C     RELAX THE OXIDE REGION.
000   C     ***********************************************************
000         DO 90 J=JJ2,K7
000         EA=3.9
000         EB=3.9
000         CALL COEFF
000         QIJ=0.
000         OMEGA=OM3
000         IF(J.GE.J3.AND.J.LE.J4) GO TO 82
000         IF(J.GE.J5.AND.J.LE.J6) GO TO 86
000         DO 80 I=2,I5
000         CALL RELAX(QIJ,OMEGA)
000      80 CONTINUE
000         CALL MAXOF
000         U(1,J)=U(I5,J)
000         GO TO 90
000      82 DO 84 I=2,I5
000         IF(I.GE.I1.AND.I.LE.I2) GO TO 84
000         IF(I.GE.I3.AND.I.LE.I4) GO TO 84
000         CALL RELAX(QIJ,OMEGA)
000      84 CONTINUE
000         CALL MAXOF
000         U(1,J)=U(I5,J)
000         GO TO 90
```

```
000      86  IL=I6+1
000          IR=I9-1
000          DO 88 I=IL,IR
000          IF(I.GE.I7.AND.I.LE.I8) GO TO 88
000          CALL RELAX(QIJ,OMEGA)
000      88  CONTINUE
000          CALL MAXOF
000          U(1,J)=U(I5,J)
000      90  CONTINUE
000     C    ***********************************************************
000     C    RELAX OXIDE-AIR INTERFACE
000     C    ***********************************************************
000          J=J7
000          EA=3.9
000          EB=1.0
000          QIJ=0.
000          OMEGA=OM3
000          DO 92 I=2,I5
000          CALL RELAX(QIJ,OMEGA)
000      92  CONTINUE
000          CALL MAXOF
000          U(1,J7)=U(I5,J7)
000     C    ***********************************************************
000     C    RELAX THE AIR-SPACE REGION.
000     C    ***********************************************************
000          DO 96 J=JJ7,K8
000          EA=1.
000          EB=1.
000          QIJ=0.
000          OMEGA=OM4
000          DO 94 I=2,I5
000          CALL RELAX(QIJ,OMEGA)
000      94  CONTINUE
000          CALL MAXOF
000          U(1,J)=U(I5,J)
000       96  CONTINUE
000          IF(ITYPE.GT.0) GO TO 99
000          DO 97 I=1,I5
000          U(I,1)=U(I,2)
000      97  CONTINUE
000      99  CONTINUE
000          WRITE(6,330) DUMAX,IMAX,JMAX
000     330  FORMAT(40X,'RMAX=',F8.3,5X,'IMAX=',I4,5X,'JMAX=',I4)
000          LWRIT=LOOP/LAP
000          IF(LWRIT.EQ.KT) GO TO  200
000      98  LOOP=LOOP+1
000          IF(LOOP.LE.ITER) GO TO 1000
000          READ(5,10) VG1,VG2,VG3,VG4,ITER,LAP
000          IF(ITER.EQ.0) STOP
000          WRITE(6,508) VG1,VG2,VG3,VG4
000          WRITE(6,510) ITER,LAP,YBAR,SIGMA
000          DO 480 J=J5,J6
000          DO 460 I=1,I5
000          U(I,J)=VG3*(F(1,I6,I)+F(I9,I5,I))+VG4*F(I7,I8,I)
000     460  CONTINUE
000     480  CONTINUE
000          DO 520 J=J3,J4
```

```
000           DO 518 I=1,I5
000           U(I,J)=VG1*F(I1,I2,I)+VG2*F(I3,I4,I)
000      518  CONTINUE
000      520  CONTINUE
000           GO TO 1000
000      200  DO 206 J=JA,JB,JC
000           WRITE(6,201) J
000      201  FORMAT(/,10X,'J=',I4/)
000           WRITE(6,202) (U(I,J),I=1,IC)
000           WRITE(6,202) (U(I,J),I=IC,I5)
000      202  FORMAT(10F10.3)
000      206  CONTINUE
000           KT=KT+1
000           IF(MAXU.GT.0) GO TO 98
000           DO 212 I=1,I5
000           UMAX=0.
000           DO 210 J=J1,J2
000           ABU=ABS(U(I,J))
000           IF(ABU.GT.UMAX) GO TO 208
000           GO TO 210
000      208  UMAX=ABU
000           JMAX=J
000      210  CONTINUE
000           DUM(I)=U(I,JMAX)
000           DU(I)=JMAX
000      212  CONTINUE
000           WRITE(6,300)
000      300  FORMAT(/,10X,'THE VALUES OF JMAX ARE:',/)
000           WRITE(6,202) (DU(I),I=1,IC)
000           WRITE(6,202) (DU(I),I=IC,I5)
000           WRITE(6,302)
000      302  FORMAT(/,10X,'THE VALUES OF UMAX ARE:',/)
000           WRITE(6,202) (DUM(I),I=1,IC)
000           WRITE(6,202) (DUM(I),I=IC,I5)
000           GO TO 98
000           END
000           FUNCTION F(II,JJ,KK)
000           F=0.0
000           IF(KK.GE.II.AND.KK.LE.JJ) F=1.0
000           RETURN
000           END
000           FUNCTION DISF(A,B,C)
000           EXPO=-((A-B)/(2.*C))**2
000           DISF=EXP(EXPO)
000           RETURN
000           END
000           SUBROUTINE COEFF
000           COMMON U(100,100),DU(100),H(100),A,B,C,G,W,EA,EB,DROW,DUMAX,QSUB
000          *,ABMAX,I,J,IMAX,JMAX,IM,I5
000           A=EA*W/H(J-1)
000           B=(EA*H(J-1)+EB*H(J))/(2.*W)
000           G=EB*W/H(J)
000           C=A+2.*B+G
000           RETURN
000           END
000           SUBROUTINE AVERO
000           COMMON U(100,100),DU(100),H(100),A,B,C,G,W,EA,EB,DROW,DUMAX,QSUB
```

```
000          *,ABMAX,I,J,IMAX,JMAX,IM,I5
000           S=0.0
000           U1=ABS(U(I,J)+U(I,J-1))
000           IF(U1.GT.0.0) S=0.5*H(J-1)
000           U2=ABS(U(I,J)+U(I,J+1))
000           IF(U2.GT.0.0) S=S+0.5*H(J)
000           QSUB=S*W
000           RETURN
000           END
000    @FORL,SI  RELAX,RELAX
000           COMMON U(100,100),DU(100),H(100),A,B,C,G,W,EA,EB,DROW,DUMAX,QSUB
000          *,ABMAX,I,J,IMAX,JMAX,IM,I5
000           UOLD=U(I,J)
000           IRITE=I+1
000           IF(I.EQ.I5) IRITE=2
000           UTIL=(A*U(I,J-1)+B*U(I-1,J)+B*U(IRITE,J)+G*U(I,J+1)+QIJ)/C
000           U(I,J)=(1.-OMEGA)*UOLD+OMEGA*UTIL
000       2   DU(I)=U(I,J)-UOLD
000           RETURN
000           END
000           SUBROUTINE MAXOF
000           COMMON U(100,100),DU(100),H(100),A,B,C,G,W,EA,EB,DROW,DUMAX,QSUB
000          *,ABMAX,I,J,IMAX,JMAX,IM,I5
000           DAB=0.0
000           DROW=0.0
000           DO 4 I=2,I5
000           ABDU=ABS(DU(I))
000           IF(ABDU.GT.DAB) GO TO 2
000           GO TO 4
000       2   DAB=ABDU
000           DROW=DU(I)
000           IM=I
000       4   CONTINUE
000           IF(DAB.GT.ABMAX) GO TO 6
000           GO TO 8
000       6   ABMAX=DAB
000           DUMAX=DROW
000           IMAX=IM
000           JMAX=J
000       8   RETURN
000           END
000    @XQT
000             16          12          16          12          1
000              5          60           5
000             30          10           5           5
000              5           5           5           5
000         0.4         0.5         0.4         0.8
000        0.8          1.0         0.5
000       2.00E+11                 4.00E+11  1.00E+15
000        5.0      20.0           -10.0                      240         80
000         1.7         1.7         1.7         1.7                 100.0
000
000    @END
000    @PCH,S   TEMP.PCH
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